

STIC Search Report

STIC Database Tracking Number: 158374

TO: Dawn Garrett

Location: REM 10C79

Art Unit : 1774 July 15, 2005

Case Serial Number: 10/680066

From: Les Henderson Location: EIC 1700 REM 4B28 / 4A30

Phone: 571-272-2538

Leslie.henderson@uspto.gov

Search Notes	- \$2 100	
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AVAILABLE COPY

SEARCH REQUEST FORM

Scientific and Technical Information Center

			<i>i</i> 1
equester's Full Name: DAW	N GARRETT	Examiner #: 76/07 Date:	7/1/2005
urt Unit: 1774 Phone Mail Box and Bldg/Room Locatio	Number 30	Serial Number:	2,066
iviali Box and Bidg/Room Locatio	n: <u>Kimsin</u> Resi 10 C 79	ults Format Preferred (circle)! APE	B DISK E-MAIL
If more than one search is subn	nitted, please prioritiz	ze searches in order of need.	*****
Please provide a detailed statement of the	search topic, and describe	as specifically as possible the subject matter	er to he searched
utility of the invention. Define any terms known. Please attach a copy of the cover	s that may have a special me	nyms, and registry numbers, and combine versing. Give examples or relevant citations abstract.	vith the concept or s, authors, etc, if
Title of Invention: Oyance	Light Emitte	no Dences with Wide	Sup /tot
Inventors (please provide full names):			Materials
<u>KLAOFAN REN. RUSSE</u>	ELL HOLIMES, S	STEPHEN FORREST, MI	ORK THOMPSON
Earliest Priority Filing Date: 4/			
For Sequence Searches Only Please inclu appropriate serial number.	/ de all pertinent information (parent, child, divisional, or issued patent num.	bers) along with the
Cla Formula VI	attacled p	leuse search	
wherein			
X is Si Y is pheny!		Sci A	IC REFERENCE BR
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		Pat.	& T.M. Office
Ar', Arza	ind Ar3 ar	e unsulatituted p	henyl
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**********	****	*******	*****
STAFF USE ONLY	Type of Search	Vendors and cost where applic	cable
earcher: XH	NA Sequence (#)	STN \$524,83	
earcher Phone #:	AA Sequence (#)	Dialog	
earcher Location:	Structure (#) 2	Questel/Orbit	·
Date Searcher Picked Up: 7/14/c5	Bibliographic	Dr.Link	·
Date Completed: 7/15/05	Litigation	Lexis/Nexis	
earcher Prep & Review Time: 30	Fulltext	Sequence Systems	·
Prep Time: 3 0	Patent Family	WWW/Internet	
mline Time: 55	Other	Other (specify)	

PTO-1590 (8-01)

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=> d his ful
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L1

L5

L6

L13

(FILE 'HOME' ENTERED AT 09:51:27 ON 15 JUL 2005)

FILE 'HCAPLUS' ENTERED AT 09:51:36 ON 15 JUL 2005 E US20040209116/PN

2 SEA ABB=ON PLU=ON US20040209116/PN D L1 1-2 ALL

SEL L1 RN

FILE 'REGISTRY' ENTERED AT 09:53:28 ON 15 JUL 2005

L2 18 SEA ABB=ON PLU=ON (159-68-2/BI OR 18849-24-6/BI OR 26393-23-7/BI OR 376367-93-0/BI OR 5256-79-1/BI OR 664374-03-2/BI OR 7439-92-1/BI OR 7440-21-3/BI OR 7440-31-5/BI OR 7440-32-6/BI OR 7440-56-4/BI OR 7440-58-6 /BI OR 7440-67-7/BI OR 7782-49-2/BI OR 94928-86-6/BI OR 18856-08-1/BI OR 18920-16-6/BI OR 550378-78-4/BI) D SCAN

FILE 'HCAPLUS' ENTERED AT 09:56:45 ON 15 JUL 2005 SEL L1 1 RN

FILE 'REGISTRY' ENTERED AT 10:00:29 ON 15 JUL 2005 D L2 1-18 RN STR

FILE 'LREGISTRY' ENTERED AT 10:05:04 ON 15 JUL 2005

Ľ3 STR

L4 STR L3

FILE 'REGISTRY' ENTERED AT 10:10:03 ON 15 JUL 2005

O SEA SSS SAM L3

D QUE STAT

O SEA SSS SAM L4

L7 SCR 1843

L8 O SEA SSS SAM L7 AND L3

D QUE STAT

D QUE STAT L5

D QUE STAT L3

D QUE STAT L5

20 SEA SSS FUL L3

D SCAN

SAV L9 GAR066/A

FILE 'HCAPLUS' ENTERED AT 10:21:49 ON 15 JUL 2005 28 SEA ABB=ON PLU=ON L9 L10

FILE 'REGISTRY' ENTERED AT 10:22:31 ON 15 JUL 2005 D OUE STAT L4

0 SEA SUB=L9 SSS SAM L4 L11

L12 13 SEA SUB=L9 SSS FUL L4 D SCAN

FILE 'HCAPLUS' ENTERED AT 10:23:44 ON 15 JUL 2005

20 SEA ABB=ON PLU=ON L12

D L13 1-20 FHITSTR

L14

8 SEA ABB=ON PLU=ON L10 NOT L13 QUE ABB=ON PLU=ON EL OR E(W)L OR L(W)E(W)D OR OLED OR L15 ELECTROLUM!N? OR ORGANOLUM!N? OR (ELECTRO OR ORGANO OR ORG#) (2A) LUM!N? OR LIGHT? (2A) (EMIT? OR EMISSION? OR SOURCE?)

QUE ABB=ON PLU=ON (LUMINES###### OR FLUORES? OR L16

PHOSPHORES?)/BI, AB OR LED/IT OR PHOSPHOR# OR LUMIN?

7 SEA ABB=ON PLU=ON L10 AND L15 L17

PLU=ON L16 AND L10 7 SEA ABB=ON L18

7 SEA ABB=ON PLU=ON L17 OR L18 L19

4 SEA ABB=ON PLU=ON L19 AND L13 L20

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L21 3 SEA ABB=ON PLU=ON L19 AND L14
L22 16 SEA ABB=ON PLU=ON L13 NOT L19
L23 5 SEA ABB=ON PLU=ON L14 NOT L19
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FILE 'REGISTRY' ENTERED AT 10:32:21 ON 15 JUL 2005 SAV L12 GAR066A/A

FILE 'HCAPLUS' ENTERED AT 10:32:58 ON 15 JUL 2005

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=> d que stat 110
L3 STR

6 8
Cb Cb
2 4
Cb Si Cb Si Cb
1 3 5
Cb Cb
7 9
```

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM GGCAT IS UNS AT GGCAT IS UNS AT 3 GGCAT IS UNS AT 5 GGCAT IS UNS AT GGCAT IS UNS AT 7 **GGCAT** IS UNS AT 8 IS UNS **GGCAT** AT9 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

L9 20 SEA FILE=REGISTRY SSS FUL L3

L10 28 SEA FILE=HCAPLUS ABB=ON PLU=ON L9

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=> d que stat 113
L3 STR

6 8
Cb Cb
2 4
Cb Si Cb Si Cb
1 3 5
Cb Cb
7 9
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NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM GGCAT IS UNS AT GGCAT IS UNS AT 3 GGCAT IS UNS ΑT 5 GGCAT IS UNS AΤ 6 GGCAT IS UNS AΤ **GGCAT** IS UNS AΤ 8 AΤ **GGCAT** IS UNS 9 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 9

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STEREO ATTRIBUTES: NONE
    6
           Cb
   Cb
     2
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NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM IS UNS AT GGCAT IS UNS **GGCAT** AT 3 GGCAT IS UNS AT 5 GGCAT IS UNS 6 AT GGCAT IS UNS AT 7 GGCAT IS UNS AT 8 GGCAT IS UNS AT DEFAULT ECLEVEL IS LIMITED ECOUNT IS E6 C AT 1 ECOUNT IS E6 C ΑT ECOUNT IS E6 C AΤ 5 ECOUNT IS E6 C AΤ 6 IS E6 C ECOUNT AT 7 IS E6 C ECOUNT AT 8 ECOUNT IS E6 C AT

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS

STEREO ATTRIBUTES: NONE

20 SEA FILE=REGISTRY SSS FUL L3 1.9

L1213 SEA FILE=REGISTRY SUB=L9 SSS FUL L4 L1320 SEA FILE=HCAPLUS ABB=ON PLU=ON L12

=> => d l19 1-7 cbib abs hitstr hitind

_application L19 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN 2004:878009 Document No. 141:372557 Organiclight emitting devices with wide gap host materials. Ren, Xiaofan; Holmes, Russell; Forrest, Stephen; Thompson, Mark E. (USA). U.S. Pat. Appl. Publ. US 2004209116 A1 20041021, 58 pp., Cont.-in-part of U.S. Ser No. 420,430. (English). CODEN: USXXCO. APPLICATION: US 2003-680066 20031006. PRIORITY: US 2003-420430 20030421.

Organic light-emitting devices having an emissive layer comprising a host material and aphosphorescent emissive material are described in which the host has a band gap ≥ 3.2 eV and a triplet energy .gtorsim.3.0 eV, and is selected from materials are described by the general formula Y-[X(Ar1)(Ar2)(Ar3)]n (X = independently selected Si, Ge, Sn, Pb, Se, Ti, Zr, and Hf; Y = Ph, alkyl, cycloalkyl, and a group of the formula Ar'-A-Ar"; Ar' and Ar" = independently selected aromatic groups; A = alkyl, cycloalkyl, -O-, or Si(R')(R"); R' and R" = independently selected Ph or alkyl; each Ar1-3 = independently selected alkyl or aromatic groups which may be independently substituted with ≥1 alkyl, alkenyl, alkoxy, Ph, aralkyl, halogen, NH, NHR, NR, SiR, and CN, and, addnl. or alternatively, ≥1 adjacent Ar1-3 may be linked together by a covalent bond, -O-, -CH, -CHR-, -CR, -NH- and -NR-; each R = alkyl, alkenyl, aryl, and aralkyl; and n = an integer between 2 up to the maximum number of sites on Y that can accept a substituent). The devices may also be provided with charge balancing layers.

IT 18856-08-1 18920-16-6

RL: DEV (Device component use); USES (Uses)
(organic light-emitting devices with emitting
layers using wide gap host materials andphosphorescent
emissive materials)

RN 18856-08-1 HCAPLUS

CN Silane, 1,4-phenylenebis (triphenyl- (9CI) (CA INDEX NAME)

RN 18920-16-6 HCAPLUS

CN Silane, 1,3-phenylenebis[triphenyl- (9CI) (CA INDEX NAME)

IC ICM H05B033-14

INCL 428690000; 428917000; 313504000; 313506000; 257040000

CC 73-11 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)

Section cross-reference(s): 29, 76

ST org light emitting device wide gap host

phosphorescent emitter

IT Electroluminescent devices

(organic; organic light-emitting devices with emitting layers using wide gap host materials and phosphorescent emissive materials)

IT 550378-78-4

RL: DEV (Device component use); USES (Uses)

(charge balancing layer; organiclight-emitting

devices with emitting layers using wide gap host materials and phosphorescent emissive materials)

IT 159-68-2, 5,5'-Spirobi(dibenzosilole) 5256-79-1 7439-92-1D,
Lead, multicenter compds. with organic mols. 7440-21-3D, Silicon,
multicenter compds. with organic mols. 7440-31-5D, Tin, multicenter
compds. with organic mols. 7440-32-6D, Titanium, multicenter compds.
with organic mols. 7440-56-4D, Germanium, multicenter compds. with
organic mols. 7440-58-6D, Hafnium, multicenter compds. with organic
mols. 7440-67-7D, Zirconium, multicenter compds. with organic mols.
7782-49-2D, Selenium, multicenter compds. with organic mols.

18849-24-6 18856-08-1 18920-16-6 26393-23-7, 9,9'(10H,10'H)-Spirobi[9-silaanthracene]

RL: DEV (Device component use); USES (Uses)

(organic light-emitting devices with emitting

layers using wide gap host materials andphosphorescent emissive materials)

94928-86-6, Tris(2-phenylpyridine)iridium 376367-93-0 664374-03-2

RL: DEV (Device component use); MOA (Modifier or additive use); USES (Uses)

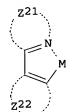
(organic light-emitting devices with emitting layers using wide gap host materials andphosphorescent emissive materials)

ΙT

L19 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN 2004:739385 Document No. 141:268179 Long-life white-emitting organic electroluminescent devices, displays, illumination apparatus, and electric appliances therewith. Fukuda, Mitsuhiro; Genda, Kazuo (Konica Minolta Holdings, Inc., Japan). Jpn. Kokai Tokkyo Koho JP 2004253298 A2 20040909, 577 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2003-43860 20030221. GI

X. date

Ι



II

The devices have, in their constituent layers (e.g., emitting layers, hole- or electron-transporting layers), (i) compds. represented by X1R1C:CR2X2 [X1, X2 = aryl, heterocycle; R1, R2 = aryl, heterocyclic hydrocarbyl, cycloalkoxy (R1 = R2 = aryl)], R11R12R13R14R15P (R11-R15 = monovalent substituent), Ar2Ar1C6H4 (m-Ar1Ar2) [Ar1 = bivalent aromatic hydrocarbylene; Ar2 = (substituted) Ph; H atom on the benzene ring may be substituted with (cyclo)alkyl, alkoxy, or halo], Z(ArQ)n [Q = (substituted) o-(2-pyridyl)phenyl; Z = n-valent bridging group, single bond; Ar = bivalent arylene; n = 2-8], etc., (ii) fluorescent compds. with mol. weight 500-2000 and atomic ratio F/(F + H) 0-0.9 and having fluorescent peak at ≤415 nm, (iii) polysilanes (R21R22Si)n [R21, R22 = alkyl(oxy), aromatic group, aryloxy; n1 ≥3] or [R31(Ar31NR32R33)Si]n [R31 = alkyl(oxy), aromatic group, aryloxy; R32, R33 = alkyl, aromatic group; Ar31 = arylene; n2 ≥3], and/or (iv) fluorescent compds. satisfying atomic ratio N/C 0-0.05. The devices, havingphosphorescent dopants I (Z11 = aromatic azacycle; Z12 = nonarom. ring, 5-membered aromatic ring, azulene; M = metal), II (Z21, Z22 = aromatic azacycle; M = metal), or III (Z41 = azacycle; Z42 = ring; M = metal) in emitting layers, are also claimed. The devices exhibit high luminescent efficiency and substantially white emission, and are suited for light source uses, especially of LCD. IT 694534-41-3

RL: DEV (Device component use); USES (Uses) (long-life white-emitting organicLED containing azacyclic phosphorescent dopants and showing high luminescent efficiency)

RN 694534-41-3 HCAPLUS

Silane, tricyclo[8.2.2.24,7] hexadeca-4,6,10,12,13,15-hexaene-5,11diylbis- (9CI) (CA INDEX NAME)

Ph₃Si

TΤ 676553-36-9P

CN

RL: DEV (Device component use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses) (long-life white-emitting organic LED containing azacyclic

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phosphorescent dopants and showing high
    luminescent efficiency)
RN 676553-36-9 HCAPLUS
CN Silane, 9,10-anthracenediylbis[triphenyl- (9CI) (CA INDEX NAME)
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ICM H05B033-14
IÇ
     ICS C09K011-06; G02F001-1335; H05B033-22
CC
     73-11 (Optical, Electron, and Mass Spectroscopy and Other Related
     Properties)
     Section cross-reference(s): 25, 28, 29, 38, 74
ST
     white emitting electroluminescent life luminescent
     efficiency; phosphorescent azacyclic dopant
     luminescent efficiency org LED; LCD light
     source white emitting electrophosphorescent
IT
     Luminescent substances
        (electroluminescent, electrophosphorescent, host-guest;
        long-life white-emitting organic LED containing azacyclic
        phosphorescent dopants and showing high
        luminescent efficiency)
     Phosphorescent substances
TТ
        (electrophosphorescent; long-life white-emitting organicLED
        containing azacyclic phosphorescent dopants and showing
        high luminescent efficiency)
IT
     Fluorescent substances
        (fluorine- or nitrogen-containing; long-life white-emitting organic
        LED containing azacyclic phosphorescent dopants and
        showing high luminescent efficiency)
TT
     Liquid crystal displays
        (light sources for; long-life white-emitting
        organic LED containing azacyclic phosphorescent
        dopants and showing highluminescent efficiency)
IT
     Electric apparatus
        (long-life white-emitting organic LED containing azacyclic
        phosphorescent dopants and showing high
```

Iuminescent efficiency)
IT Organometallic compounds
Polysilanes

RL: DEV (Device component use); USES (Uses)
(long-life white-emitting organicLED containing azacyclic phosphorescent dopants and showing high

luminescent efficiency)

IT Electroluminescent devices
 (white-emitting, electrophosphorescent; long-life white-emitting organic LED containing azacyclic phosphorescent

dopants and showing high luminescent efficiency)

IT 159-68-2, 9,9'-Spirobi[9H-9-silafluorene] 71-43-2, Benzene, uses 752-28-3 1423-70-7 17742-49-3 18822-13-4 346-02-1 38186-32-2 20156-53-0 32314-41-3 33861-11-9 35088-77-8 54765-15-0 65181-79-5 122107-04-4 133942-93-5 139376-06-0 142289-08-5 203070-80-8 219917-71-2 213621-16-0 288581-17-9 300823-56-7 300823-57-8 301300-11-8 332350-53-5 405171-49-5 405171-87-1 405172-39-6 453590-51-7 478262-73-6 478262-74-7 478262-76-9 478262-77-0 478262-78-1 478262-79-2 478370-42-2 492446-94-3 492446-97-6 497097-34-4 497097-36-6 511270-11-4 522630-08-6 522630-12-2 522630-19-9 522630-30-4 522630-34-8

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     754231-91-9
                   754231-92-0
                                  754231-94-2
     RL: DEV (Device component use); USES (Uses)
        (long-life white-emitting organicLED containing azacyclic
        phosphorescent dopants and showing high
        luminescent efficiency)
TT
     5660-43-5P
                                 115533-27-2P
                  51445-93-3P
                                                174291-37-3P
     288297-90-5P
                    344564-96-1P
                                    522630-06-4P
                                                   522630-07-5P
     557787-52-7P
                    567625-71-2P
                                    567625-76-7P
                                                   567625-77-8P
     569674-88-0P
                    569674-97-1P
                                    643753-84-8P
                                                   669072-95-1P
     676553-36-9P
                    705941-83-9P
                                    754231-93-1P
                                                   754231-95-3P
     754232-01-4P
                    754980-36-4P
     RL: DEV (Device component use); IMF (Industrial manufacture); PREP
     (Preparation); USES (Uses)
        (long-life white-emitting organic LED containing azacyclic
        phosphorescent dopants and showing high
        luminescent efficiency)
TТ
     604-53-5P, 1,1'-Binaphthalene
                                      5122-94-1P
                                                   16761-23-2P
                                                50668-21-8P,
     19264-73-4P
                  33170-68-2P 49610-33-5P
     3-Iodo-9-ethylcarbazole
                               77547-84-3P
                                              85137-69-5P
                                                             103989-84-0P
     121073-89-0P
                    146232-42-0P
                                    155886-75-2P
                                                   155886-83-2P
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                    288297-93-8P
                                    288297-94-9P
                                                   288297-95-0P
     357437-74-2P
                    363607-69-6P
                                    522630-41-7P
                                                   522630-42-8P
     567625-82-5P
                    567625-83-6P
                                    643753-87-1P
                                                   643753-91-7P
     754232-02-5P
     RL: IMF (Industrial manufacture); RCT (Reactant); PREP
     (Preparation); RACT (Reactant or reagent)
        (long-life white-emitting organic LED containing azacyclic
        phosphorescent dopants and showing high
        luminescent efficiency)
IT
     62-53-3, Aniline, reactions
                                   67-64-1, Acetone, reactions
                                                                   76-86-8,
                             86-74-8, Carbazole
     Triphenylchlorosilane
                                                   90-11-9,
     1-Bromonaphthalene
                         90-90-4, 4-Bromobenzophenone
                                                          92-66-0.
     4-Bromobiphenyl
                      95-54-5, 1,2-Phenylenediamine, reactions
                                    99-97-8, N,N-Dimethyl-p-tolylamine
     98-80-6, Phenylboronic acid
     100-20-9, Terephthaloyl dichloride 106-37-6, 1,4-Dibromobenzene
     106-38-7, 4-Bromotoluene
                                108-36-1, 1,3-Dibromobenzene
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Cyclohexanone, reactions
                           108-98-5, Thiophenol, reactions
110-13-4, 2,5-Hexanedione
                           119-61-9, Benzophenone, reactions
119-93-7
          121-43-7, Trimethoxyborane
                                       132-32-1,
3-Amino-9-ethylcarbazole
                           302-01-2, Hydrazine, reactions
495-71-6, 1,2-Dibenzoylethane
                               523-27-3, 9,10-Dibromoanthracene
583-53-9, 1,2-Dibromobenzene 623-27-8, 1,4-Diformylbenzene
                               619-42-1, Methyl 4-bromobenzoate
                                624-92-0, Dimethyl disulfide
626-19-7, 1,3-Benzenedicarboxaldehyde
                                        762-04-9, Diethyl phosphite
826-81-3, 2-Methyl-8-quinolinol
                                  885-39-2
                                             931-50-0,
Cyclohexylmagnesium bromide
                              1003-09-4, 2-Bromothiophene
1074-24-4, 2,5-Dibromo-p-xylene
                                  1592-95-6, 3-BromoCarbazole
1730-04-7, 1,8-Diiodonaphthalene
                                   1733-63-7
                                                2586-62-1,
1-Bromo-2-methylnaphthalene
                              2592-73-6, 1,1-Dibromo-2,2-
                               6999-03-7, 1-Bromo-4-
diphenylethylene 4546-04-7
trimethylsilylbenzene
                       10489-97-1, 1,1-Dibromocyclohexane
38218-24-5, Indium isopropoxide
                                  51044-13-4, 4-
                                         65810-18-6,
Bromobenzyltriphenylphosphonium bromide
1,3,5-Cycloheptatriene-1-carboxaldehyde
                                           95902-10-6,
3-Bromobenzyltriphenylphosphonium bromide 643753-90-6
754232-00-3
RL: RCT (Reactant); RACT (Reactant or reagent)
   (long-life white-emitting organic LED containing azacyclic
  phosphorescent dopants and showing high
   luminescent efficiency)
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L19 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
2004:711217 Document No. 141:372479 Ultrahigh Energy Gap Hosts in Deep
Blue Organic Electrophosphorescent Devices. Ren, Xiaofan; Li, Jian;
Holmes, Russell J.; Djurovich, Peter I.; Forrest, Stephen R.;
Thompson, Mark E. (Department of Chemistry, University of Southern
California, Los Angeles, CA, 90089, USA). Chemistry of Materials,
16(23), 4743-4747 (English) 2004. CODEN: CMATEX. ISSN: 0897-4756.

X-date

Publisher: American Chemical Society. AB Four ultrahigh energy gap organosilicon compds. [diphenyldi(otolyl) silane (UGH1), p-bis(triphenylsilyl) benzene (UGH2), m-bis(triphenylsilyl)benzene (UGH3), and 9,9'-spirobisilaanthracene (UGH4)] were employed as host materials in the emissive layer of electrophosphorescent organiclight-emitting diodes (OLEDs). The high singlet (.apprx.4.5 eV) and triplet (.apprx.3.5 eV) energies associated with these materials effectively suppress both the electron and energy transfer quenching pathways between the emissive dopant and the host material, leading to deep blue phosphorescent devices with high (.apprx.10%) external quantum efficiencies. Also, by direct charge injection from the adjacent hole and electron transport layers onto the phosphor doped into the UGH matrix, exciton formation occurs directly on the dopant, thereby eliminating exchange energy losses characteristic of guest-host energy transfer. The authors discuss the material design, and present device data forOLEDs employing UGHs. Among the 4 host materials, UGH2 and UGH3 have higher quantum efficiencies than UGH1 when used inOLEDs: Rapid device degradation was observed for the UGH4-based device due to electro- and/or photooxidn. of the diphenylmethane moiety in UGH4. In addition to showing that UGH materials can be used to fabricate efficient blue OLEDs, very high device efficiencies can be achieved in structures where the dopant transports both charge and excitons.

IT 18856-08-1, p-Bis(triphenylsily1)benzene 18920-16-6
, m-Bis(triphenylsily1)benzene
RL: DEV (Device component use); USES (Uses)

(ultrahigh energy gap hosts in deep blue organic electrophosphorescent devices containing)

RN 18856-08-1 HCAPLUS

CN Silane, 1,4-phenylenebis[triphenyl- (9CI) (CA INDEX NAME)

18920-16-6 HCAPLUS RN

Silane, 1,3-phenylenebis[triphenyl- (9CI) (CA INDEX NAME) CN

73-11 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)

Section cross-reference(s): 72, 74, 76

ST electrophosphorescent device organosilicon blue ultrahigh energy gap host; LED organosilicon blue ultrahigh energy gap host; silicon org deriv electrophosphorescent device blue ultrahigh gap host; luminescence silicon org deriv

electrophosphorescent device blue; thermooptical

luminescence silicon org deriv

electrophosphorescent device blue; UV spectra silicon org deriv electrophosphorescent device blue; current voltage silicon org deriv electrophosphorescent device blue; photooxidn silicon org deriv electrophosphorescent device blue; electrochem oxidn silicon org deriv electrophosphorescent device blue; band gap silicon org deriv electrophosphorescent device blue; energy level silicon org deriv electrophosphorescent device blue

IT Luminescence

> (UV; of organosilicon derivative for deep blue organic electrophosphorescent devices)

IT Electroluminescent devices

> (blue-emitting; ultrahigh energy gap hosts in deep blue organic electrophosphorescent devices)

IT Thermooptical effect

> (luminescence; of organosilicon derivative for deep blue organic electrophosphorescent devices)

IT Band gap

Energy level

Luminescence

UV and visible spectra

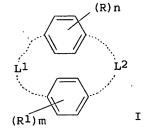
(of organosilicon derivative for deep blue organic electrophosphorescent devices)

IT 4733-39-5, 2,9-Dimethyl-4,7-diphenyl-1,10phenanthroline 18856-08-1, p-Bis(triphenylsilyl)benzene **18920-16-6**, m-Bis(triphenylsilyl)benzene 123847-85-8 550378-78-4, N,N'-Dicarbazolyl-3,5-benzene RL: DEV (Device component use); USES (Uses) (ultrahigh energy gap hosts in deep blue organic electrophosphorescent devices containing)

L19 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN 427863 Document No. 141:14542 Organicelectroluminescent devices and displays using them. Kita, Hiroshi; Yamada, Taketoshi; 2004:427863 Ueda, Noriko; Fukuda, Mitsuhiro (Konica Minolta Holdings Inc.,

Japan). Jpn. Kokai Tokkyo Koho JP 2004152527 A2 20040527, 37 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2002-314134 20021029.

GI



AB The devices include paracyclophanes I (R, R1 = substituent; L1, L2 = bivalent linkage; m, n = 0-4; plural R may form ring when n≥2; plural R1 may form ring when m≥2). The devices and displays show high luminescence intensity and efficiency, and long service life.

694534-41-3

RL: DEV (Device component use); USES (Uses) (emitters; organic electroluminescent devices and displays including paracyclophanes) 694534-41-3 HCAPLUS

RN

Silane, tricyclo[8.2.2.24,7] hexadeca-4,6,10,12,13,15-hexaene-5,11-CN (CA INDEX NAME) diylbis- (9CI)



IC ICM H05B033-14 ICS C09K011-06

74-13 (Radiation Chemistry, Photochemistry, and Photographic and CC Other Reprographic Processes) Section cross-reference(s): 73

ST org electroluminescent device paracyclophane; paracyclophane orgelectroluminescent display; carbazolyl paracyclophane orgelectroluminescent display

IT Electroluminescent devices

(displays; organic electroluminescent devices and displays including paracyclophanes)

IT Luminescent screens

(electroluminescent; organic

electroluminescent devices and displays including paracyclophanes)

IT Electroluminescent devices

> (organic electroluminescent devices and displays including paracyclophanes)

IT Cyclophanes

IT

RL: DEV (Device component use); USES (Uses)

(paracyclophanes; organicelectroluminescent devices and displays including paracyclophanes)

IT 94928-86-6 343978-79-0 376367**-**93-0

RL: DEV (Device component use); MOA (Modifier or additive use); USES (Uses)

(dopants in emitter layers; organicelectroluminescent devices and displays including paracyclophanes)

694534-48-0 694534-49**-**1 694534-50-4 694534-51-5

RL: DEV (Device component use); USES (Uses)

(electron transporters; organicelectroluminescent devices and displays including paracyclophanes)

IT 694534-38-8

RL: DEV (Device component use); USES (Uses)
(emitters or electron transporters; organic
electroluminescent devices and displays including
paracyclophanes)

IT 694534-34-4 694534-35-5 694534-36-6 694534-37-7 694534-39-9 694534-40-2 694534-41-3 694534-42-4 694534-43-5 694534-44-6 694534-45-7 694534-46-8 694534-47-9 RL: DEV (Device component use); USES (Uses)

(emitters; organic electroluminescent devices and displays including paracyclophanes)

L19 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

2004:371815 Document No. 141:147748 Efficient organic
electrophosphorescent white light-emitting
device with a triple doped emissive layer. D'Andrade, Brian W.;
Holmes, Russell J.; Forrest, Stephen R. (Department of Electrical
Engineering, Princeton University, Princeton, NJ, 08544, USA).
Advanced Materials (Weinheim, Germany), 16(7), 624-628 (English)
2004. CODEN: ADVMEW. ISSN: 0935-9648. Publisher: Wiley-VCH Verlag

X- date

GmbH & Co. KGaA.

A high efficiency white organic LED with a thin electrophosphorescent triple doped host and efficient exciton and charge confinement is demonstrated. Devices haveηp = 14 ± 1 lm W-1 at 10 mA cm-2, a maximum η1 = 42 ± 4 lm W-1 and CIE coordinates that vary from [0.43,45] at 0.1 mA cm-2 to [0.38,0.45] at 10 mA cm-2, with CRI = 80. The device emission color is effectively controlled by varying dopant concns. As in the case of recently reported deep-blue-emitting electrophosphorescentOLEDs, high efficiency is obtained by direct triplet formation on the blue dopant by near-resonant charge transfer from nearby charge injection layers, avoiding exchange energy losses incurred by energy transfer from a singlet exciton state in the host to a triplet state in the phosphore.

IT 18856-08-1

RL: DEV (Device component use); USES (Uses)
(efficient organic electrophosphorescent whiteLED with
triple doped emissive layer containing)

RN 18856-08-1 HCAPLUS

CN Silane, 1,4-phenylenebis[triphenyl- (9CI) (CA INDEX NAME)

CC 73-11 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)

Section cross-reference(s): 76

electrophosphorescent white light emitting
device triple doped emissive layer; LED white electrophosphorescent
triple doped emissive layer

IT Electroluminescent devices

(organic; efficient electrophosphorescent whiteLED with triple doped emissive layer)

IT 18856-08-1 139092-78-7 192198-85-9, 1,3,5-Tris(Nphenylbenzimidazol-2-yl) benzene

RL: DEV (Device component use); USES (Uses)

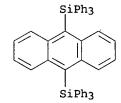
(efficient organic electrophosphorescent whiteLED with triple doped emissive layer containing)

IT 94928-86-6, fac-Tris(2-phenylpyridine)iridium 337526-95-1
RL: DEV (Device component use); MOA (Modifier or additive use); USES
(Uses)

(efficient organic electrophosphorescent whiteLED with triple doped emissive layer containing)

- L19 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

 2004:272156 Document No. 140:312148 Organicelectroluminescent
 device and electroluminescent display. Kita, Hiroshi;
 Suzurizato, Yoshiyuki; Yamada, Taketoshi; Karatsu, Takashi;
 Kitamura, Akihide (Konica Minolta Holdings Inc., Japan). Jpn. Kokai
 Tokkyo Koho JP 2004103463 A2 20040402, 23 pp. (Japanese). CODEN:
 JKXXAF. APPLICATION: JP 2002-265416 20020911.
- AB The title device contains specific triphenylarylsilane in an electroluminescent layer. The silane compound is used a host compound or an electron transporting compound. The title device shows improved electroluminescence and high durability.
- CN Silane, 9,10-anthracenediylbis[triphenyl- (9CI) (CA INDEX NAME)



- IC ICM H05B033-14 ICS C09K011-06; H05B033-22; C07F007-08; C07F007-10
- CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
 Section cross-reference(s): 29, 73
- ST org electroluminescent device display aryl silane
- IT Silanes
 - RL: TEM (Technical or engineered material use); USES (Uses) (aryl; silane compound in organicelectroluminescent device)
- IT Electroluminescent devices
 - (displays; organic electroluminescent device and electroluminescent display)
- IT Luminescent screens
 - (electroluminescent; organic
 - electroluminescent device and electroluminescent
 display)
- IT Electroluminescent devices
 - (organic electroluminescent device and electroluminescent display)
- IT 676553-36-9 676553-37-0 676553-38-1 676553-39-2
 676553-40-5 676553-41-6 676553-42-7 676553-43-8 676553-44-9
 RL: TEM (Technical or engineered material use); USES (Uses)
 (silane compound in organicelectroluminescent device)
- L19 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

 2003:859655 Document No. 140:66970 Efficient, deep-blue organic electrophosphorescence by guest charge trapping. Holmes, R. J.; D'Andrade, B. W.; Forrest, S. R.; Ren, X.; Li, J.; Thompson, M. E. (Department of Electrical Engineering and the Princeton Materials Institute, Center for Photonics and Optoelectronic Materials (POEM), Princeton University, Princeton, NJ, 08544, USA). Applied Physics Letters, 83(18), 3818-3820 (English) 2003. CODEN: APPLAB. ISSN: 0003-6951. Publisher: American Institute of Physics.
- AB Efficient, deep-blue organic electrophosphorescence was demonstrated using a charge-trapping phosphorescent guest, Ir(III)

Publication Potate 3,2063 November 3,2063 bis (4',6'-difluorophenylpyridinato) tetrakis (1-pyrazolyl) borate (FIr6) doped in the wide-energy-gap hosts, diphenyldi (o-tolyl) silane (UGH1) and p-bis (triphenylsilyl) benzene (UGH2), where exciton formation occurs directly on the guest mols. Charge trapping on the guest is confirmed by the dependence of the drive voltage and electroluminescence spectrum on guest concentration UV photoemission spectroscopy measurements establish the relative HOMO positions of FIr6 in UGH1 and UGH2. Peak quantum and power efficiencies of (8.8 ± 0.9) % and (11.0 ± 1.1) lm/W in UGH1 and (11.6 ± 1.2) % and (13.9 ± 1.4) lm/W in UGH2 are obtained, while the emission in both cases is from FIr6 and is characterized by Commission Internationale de l'Eclairage coordinates of (x = 0.16, y = 0.26) in UGH2.

IT 18856-08-1

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process) (efficient deep-blue organic electrophosphorescence by guest charge trapping using)

RN 18856-08-1 HCAPLUS

CN Silane, 1,4-phenylenebis[triphenyl- (9CI) (CA INDEX NAME)

CC 73-5 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)

Section cross-reference(s): 76

ST electrophosphorescence deep blue org guest charge trapping;
phosphorescence electro deep blue org guest charge trapping
IT Phosphorescence

(electro-, deep blue; efficient deep-blue organic electrophosphorescence by guest charge trapping)

IT Luminescence

UV photoelectron spectra

(of bis(triphenylsily1)benzene and diphenylditolylsilane and iridium bis(difluorophenylpyridinato)tetrakis(pyrazoly1)borate)

IT 18849-24-6 18856-08-1

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process) (efficient deep-blue organic electrophosphorescence by guest charge trapping using)

=> => d 122 1-16 cbib abs hitstr hitind

L22 ANSWER 1 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

1995:408011 Document No. 122:293462 Novel organosilane crosslinking
agents for powder coatings. Thames, S. F.; Panjnani, K. G.; Pace,
S. D.; Blanton, M. D.; Cumberland, B. R. (Univ. South. Mississippi,
Hattiesburg, MS, 39406-0076, USA). Journal of Coatings Technology,
67(841), 39-45 (English) 1995. CODEN: JCTEDL. ISSN: 0361-8773.
Publisher: Federation of Societies for Coatings Technology.

AB Organosilanedicarboxylic acids have been substituted for a portion
of the carboxyl-terminated polyesters in conventional
epoxy-polyester powder coatings and provide improvements in a number of
performance characteristics. For instance, environmental SEM
studies confirm improvements in flow and leveling; the modified
powders permit lower cure temps.; and chemical and weather resistance

properties are improved as is their thermal stability. Adhesion and pencil hardness are essentially unchanged, but minor improvements are noted in some formulations. However, impact strength and

flexibility are lowered for most silane-containing formulations, probably a consequence of higher aromatic content in the silane diacids.

IT 163356-34-1, 2,5-Bis(triphenylsilyl)terephthalic
 acid-Cargill 30-3051-Epon 2002-Epon 1001F copolymer
 RL: PRP (Properties); TEM (Technical or engineered material use);
 USES (Uses)

(organosilanedicarboxylic acid crosslinking agents for epoxy-polyester powder coatings)

RN 163356-34-1 HCAPLUS

1,4-Benzenedicarboxylic acid, 2,5-bis(triphenylsilyl)-, polymer with 1,4-benzenedicarboxylic acid, (chloromethyl)oxirane, 2,2-dimethyl-1,3-propanediol, Epon 2002 and 4,4'-(1-methylethylidene)bis[phenol] (9CI) (CA INDEX NAME)

CM 1

CN

CRN 163356-33-0 CMF C44 H34 O4 Si2

CM 2

CRN 126-30-7 CMF C5 H12 O2

$$\begin{array}{c} \text{Me} \\ | \\ \text{HO-CH}_2\text{-C-CH}_2\text{-OH} \\ | \\ \text{Me} \end{array}$$

CM 3

CRN 106-89-8 CMF C3 H5 Cl O

CM 4

CRN 100-21-0 CMF C8 H6 O4

CM 5

CRN 80-05-7 CMF C15 H16 O2

42-9 (Coatings, Inks, and Related Products) 163356-23-8, Cargill 30-3051-Epon 2002-Epon 1001F-2-CC IT trimethylsilylterephthalic acid copolymer 163356-24-9, 2-(Dimethylphenylsilyl)terephthalic acid-Cargill 30-3051-Epon 2002-Epon 1001F copolymer 163356-26-1, 2-(Diphenylmethylsilyl)terephthalic acid-Cargill 30-3051-Epon 2002-Epon 1001F copolymer 163356-27-2, Cargill 30-3051-Epon 2002-Epon 1001F-2-triphenylsilylterephthalic acid copolymer 163356-28-3, 2,5-Bis(trimethylsilyl)terephthalic acid-Cargill 30-3051-Epon 2002-Epon 1001F copolymer 163356-30-7, 2,5-Bis(dimethyphenylsilyl)terephthalic acid-Cargill 30-3051-Epon 2002-Epon 1001F copolymer 163356-32-9, 2,5-Bis(diphenylmethylsilyl)terephthalic acid-Cargill 30-3051-Epon 2002-Epon 1001F copolymer 163356-34-1, 2,5-Bis(triphenylsilyl)terephthalic acid-Cargill 30-3051-Epon 2002-Epon 1001F copolymer RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses) (organosilanedicarboxylic acid crosslinking agents for epoxy-polyester powder coatings)

L22 ANSWER 2 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

1993:169160 Document No. 118:169160 EPR spectra of sterically hindered silicon-containing phenoxyls. Klimov, E. S.; Muslin, D. V.; Lyapina, N. Sh.; Shpakov, A. V.; Okhlobystin, O. Yu. (NII Khim. Svobod. Radikalov, Vladikavkaz, Russia). Teoreticheskaya i Eksperimental'naya Khimiya, 28(1), 67-72 (Russian) 1992. CODEN: TEKHA4. ISSN: 0497-2627.

Ι

AB ESR spectral parameters for title compds. I (R = R1 = Me, Et; R = Me, R1 = Et, OMe, OEt, OCHMe2, OCMe3; R = Et, R1 = Me) are reported:

splitting consts. for unpaired electrons on meta protons on the aromatic phenoxyl ring, on protons of the organosilyl groups and on magnetic silicon nuclei, and g-factor values. The stability of silicon-containing phenoxyls relative to each other was determined. The effect of a second Si-containing substituent in the ortho position and of an alkyl substituent in the para position was traced in spectra of 2,6-bis(triphenylsilyl)-4-tert-butylphenoxyl and 2,6-bis(trimethylsilyl)-4-ethylphenoxyl radicals. Stability of the aroxyls is determined mostly by steric screening of the radical center responsible for dimerization-rearrangement reactions.

IT 145249-90-7P

RL: PREP (Preparation) (formation and ESR of)

RN 145249-90-7 HCAPLUS

CN Phenoxy, 4-(1,1-dimethylethyl)-2,6-bis(triphenylsilyl)- (9CI) (CA INDEX NAME)

IT 91666-25-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and oxidation of, phenoxyl radical by)

RN 91666-25-0 HCAPLUS

CN Phenol, 4-(1,1-dimethylethyl)-2,6-bis(triphenylsilyl)- (9CI) (CA INDEX NAME)

CC 29-6 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22

IT 5920-86-5P 75292-30-7P 75292-31-8P 75292-32-9P 145249-86-1P 145249-87-2P 145249-88-3P 145249-89-4P**145249-90-7P**

145273-37-6P RL: PREP (Preparation)

(formation and ESR of)

IT 91666-25-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and oxidation of, phenoxyl radical by)

L22 ANSWER 3 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

1987:5154 Document No. 106:5154 Radical ions. 70. The effect of
 phosphorus substituents on the cyclic voltammetric reduction of
 aromatic π-systems. Bock, Hans; Lechner-Knoblauch, Ulrike;
 Haenel, Peter (Inst. Anorg. Chem., Univ. Frankfurt, Frankfurt/Main,
 D-6000/50, Fed. Rep. Ger.). Chemische Berichte, 119(12), 3749-65
 (German) 1986. CODEN: CHBEAM. ISSN: 0009-2940. OTHER SOURCES:
 CASREACT 106:5154.

AB The half-wave reduction potentials of 23 organophosphorus compds. R(PR12)n, R(P+R13)n, and R(PYR12) (R = benzene, biphenyl, naphthalene, thiophene, styrene, phenylacetylene, ferrocene; R1 =

Me, Ph; Y = O, S, Se, NR; n = 1,2) are determined by cyclic voltammetry (CV) in DMF under aprotic conditions. Statistical anal. with a π -perturbation model and comparison with the CV data of other 1,4-disubstituted benzene derivs. establishes the following sequence of increasing acceptor ability of the substituents: PMe2 « SiMe3 < PPh2 < P(O)Me2 < P(S)Me2 \approx P(NR)Me2 \approx $P(Se)Me2 \approx CN < P+Me3 \ll BR2 < P+Ph3 \ll NO2.$

IT 18856-08-1

> RL: RCT (Reactant); RACT (Reactant or reagent) (electrochem. reduction of)

RN 18856-08-1 HCAPLUS

CN Silane, 1,4-phenylenebis[triphenyl- (9CI) (CA INDEX NAME)

IT

29-7 (Organometallic and Organometalloidal Compounds) CC

Section cross-reference(s): 22, 72

100-25-4 603-35-0, Triphenylphosphine, reactions 623-26-7 1179-06-2 1707-00-2, Dimethylphenylphosphine sulfide 2633-26-3 3878-45-3, Triphenylphosphine sulfide 7016-58-2 10498-57-4, 1,4-Bis(dimethylphosphino)benzene 12150-46-8 13991-08-7 77876-83-6 **18856-08-1** 69220-11-7 77876-82-5 77876-84-7 82340-10-1 82340-11-2 82340-12-3 82340-14-5 87319-71-9 103693-23-8 103693-24-9 103693-25-0 103693-26-1 103693-27-2 103693-28-3D, derivs. RL: RCT (Reactant); RACT (Reactant or reagent) (electrochem. reduction of)

L22 ANSWER 4 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN 1984:503306 Document No. 101:103306 High-performance liquid chromatography of organometallic compounds. Ermoshkin, A. E.; Makarenko, N. P.; Sakodynskii, K. I. (Inst. Chem., Gorkiy, 603137, USSR). Journal of Chromatography, 290, 377-91 (English) 1984. CODEN: JOCRAM. ISSN: 0021-9673.

AΒ High-performance liquid chromatog. (HPLC) was applied to the separation and determination of organometallic compds. (OMC) of the following classes: (1) sterically hindered Si-containing phenols and some of their alkyl-substituted analogs; (2) silyl-, alkyl- and Br-substituted naphthalenes; (3) tri- and pentaphenyl derivs. of P, Sb, and Bi; and (4) ferrocenyl and cymantrenyl derivs. of Sb and Bi. Optimal separation conditions were determined and the main retention regularities on Silochrom C-80 and Silasorb 600, when using hexane containing 0-3 volume% Et20 as the eluent, are discussed. Examples of the separation and anal. of reaction and artificial mixts. of OMC with similar structures carried out by normal-phase HPLC are given. Substituent effects and correlations with spectral frequencies of the naphthalene-(NC) 2C:C(CN) 2 charge-transfer complexes are also discussed.

ŀΤ 91666-25-0

> RL: ANST (Analytical study); PROC (Process) (separation of, from organometallic compds., HPLC)

RN 91666-25-0 HCAPLUS

Phenol, 4-(1,1-dimethylethyl)-2,6-bis(triphenylsilyl)- (9CI) CN INDEX NAME)

CC 80-4 (Organic Analytical Chemistry) Section cross-reference(s): 22 IT 71-43-2, analysis 88-18-6 90-11 93-04-9 96-76-4 102-54-5 128-

90-11-9 91-20-3, analysis 91-57-6 573-97-7 96-76-4 128-39-2 497-39-2 93-04-9 102-54-5 607-58-9 603-35-0, analysis 603-33-8 603-36-1 616-55-7 2170-05-0 2588-88-7 3401-47-6 12079-65-1 732-26-3 791-28-6 13328-67-1 15288-53-6 16239-18-2 18033-63-1 18081-08-8 20834-61-1 27008-35-1 27329-77-7 33307-27-6 41908-23-0 50738-39-1 50738-43-7 . 53553-74-5 53553-76-7 53553-78-9 55454-56-3 55454-57-4 55454-58-5 54863-82-0 58144-48-2 58933-96-3 63247-81-4 67044-81-9 70508-60-0 75315-02-5 75333-72-1 91608-07-0 91608-08-1 91608-09-2 91649-32-0 91666-18-1 91666-19-2 91666-22-7 91666-20-5 91666-21-6 91666-23-8 91666-24-9 91666-25-0 91666-26-1

RL: ANST (Analytical study)

(separation of, from organometallic compds., HPLC)

L22 ANSWER 5 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

1976:5057 Document No. 84:5057 Preparation and thermal behavior of some polyarylsilanes. El-Attar, Azza A. A.; Cerny, M. (Inst. Chem. Process Fundam., Czech. Acad. Sci., Prague-Suchdol, Czech.). Collection of Czechoslovak Chemical Communications, 40(9), 2806-15 (English) 1975. CODEN: CCCCAK. ISSN: 0010-0765.

AB Bifunctional Ph3Si, Ph2(MeO)Si, Ph2(EtO)Si, and Ph2MeSi derivs. of C6H14, C6H6, Ph2, and Ph2O were prepared and their volatility and oxidation stability on heating under N or in air determined by thermogravimetric anal. (P-Ph3SiC6H4)2 and (p-Ph3SiC6H4)2O were more stable at elevated temps. than some com. stationary phases for gas-chromatog.

IT 18856-08-1P 18920-16-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and thermal behavior of, gas chromatog. in relation to)

RN 18856-08-1 HCAPLUS

CN Silane, 1,4-phenylenebis[triphenyl- (9CI) (CA INDEX NAME)

RN 18920-16-6 HCAPLUS

CN Silane, 1,3-phenylenebis[triphenyl- (9CI) (CA INDEX NAME)

CC 29-6 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 66

IT 18826-13-6P 18856-08-1P 18920-16-6P 47856-57-5P 57519-23-0P , 57519-24-1P 57519-25-2P 57519-26-3P

57519-27-4P 57519-28-5P 57519-29-6P 57519-30-9P 57519-31-0P 57519-32-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and thermal behavior of, gas chromatog. in relation to)

- L22 ANSWER 6 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN 1973:28877 Document No. 78:28877 Anion radicals of phenylsilanes. Wan, Yieh-Ping; O'Brien, Daniel H.; Smentowski, Frank J. (Dep. Chem., Texas A and M Univ., College Station, TX, USA). Journal of the American Chemical Society, 94(22), 7680-6 (English) 1972. CODEN: JACSAT. ISSN: 0002-7863.
- The anion radicals of phenylsilanes containing both H and Me attached to Si were characterized by ESR. These anion radicals, especially ones AR containing Si-H bond(s), showed only limited stability and further reduction gave other paramagnetic species. Identification of the anion radicals resulting from further reduction showed that 3 modes of reaction occurred: (a) para coupling with the formation of 1,4-bis(disily1)benzene anion radicals and then formation of tetraphenylsilane anion radical; (b) formation of biphenyl anion radical from diphenylsilanes; or (c) reaction with MeOCH2CH2OMe to form phenyltrimethylsilane anion radical.
- TT 40491-34-7

RL: PRP (Properties)

(ESR of)

RN 40491-34-7 HCAPLUS

Silane, 1,4-phenylenebis[triphenyl-, radical ion(1-) (9CI) (CA INDEX NAME)

CC 22-4 (Physical Organic Chemistry)

34525-07-0 IT 34471-35-7 34519-00-1 34519-02-3 34525-05-8 34536-81-7 40491-32-5 40491-33-640491-34-7 40491-35-8 40491-36-9 40491-37-0 40491-38-1 RL: PRP (Properties)

(ESR of)

- L22 ANSWER 7 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN 1968:477326 Document No. 69:77326 Polyhalo-organometallic and -organometalloidal compounds. XXII. The reaction of triphenylsilyllithium with hexafluorobenzene. Fearon, F. W. Gordon; Gilman, Henry (Iowa State Univ., Ames, IA, USA). Journal of Organometallic Chemistry, 13(1), 73-80 (English) 1968. JORCAI. ISSN: 0022-328X.
- The reaction of triphenylsilyllithium (I) with an excess of AB hexafluorobenzene at low temps. gave hexaphenyldisilane (II) and 1,4-bis(triphenylsilyl)tetrafluorobenzene instead of the expected (pentafluorophenyl)triphenylsilane. In an attempt to account for the formation of these products, the reactions of I with certain organosilicon-substituted polyfluorobenzenes were investigated and described. In contrast to the above reactions, I reacted with hexachlorobenzene via halogenmetal exchange to give pentachlorophenyllithium and II.
- IT 20083-04-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 20083-04-9 HCAPLUS

Silane, (2,3,5,6-tetrafluoro-p-phenylene)bis[triphenyl- (8CI) CN INDEX NAME)

29 (Organometallic and Organometalloidal Compounds) CC IT 789-25-3DP, Silane, triphenyl-, lithium complex 1450-23-3P 20083-04-9P 20083-06-1P 20083-07-2P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

L22 ANSWER 8 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN 1964:484352 Document No. 61:84352 Original Reference No. 61:14700e-h,14701a Group IV organometallic chemistry. XVI. Synthesis of organogermanium compounds containing the p-phenylene group. Some infrared characteristics of p-phenylene derivatives of Si, Ge, Sn, and Pb. Leusink, A. J.; Noltes, J. G.; Budding, H. A.; van der Kerk, G. J. M. (TNO Utrecht, Neth.). Recueil des Travaux Chimiques des Pays-Bas, 83(8), 844-56 (English) 1964. CODEN: RTCPA3. ISSN: 0165-0513. OTHER SOURCES: CASREACT 61:84352. cf. CA 61, 13149e. To p-ClC6H4MgCl (I) [from 4.9 g. Mg and 29.4 g. AB p-ClC6H4Cl (II) in 60 ml. tetrahydrofuran (THF)] was added dropwise 31.6 g. Me3GeBr and the whole refluxed 6 hrs. and decomposed with dilute HCl to give 17.5 g. Me3GeC6H4Cl-p, bl2 108-14°, n20D 1.5241. To p-ClC6H4Li (from 0.3 mole BuLi and 0.3 mole p-ClC6H4Cl in 315 ml. Et20) was added dropwise 17.4 g. Me2GeCl2 (III) to give as above 17.4 g. Me2Ge(C6H4Cl-p)2 (IV), b0.02 142-4°. To I (from 2.83 g. Mg, 17.0 g. II, and 60 ml. THF was added dropwise 22.1 g. III in 100 ml. THF to give p-ClC6H4GeMe2Cl, b12 116-18°, n2OD 1.5512. To 34.7 g. III in 70 ml. THF was added dropwise p-BrMgC6H4MgBr (IVa) (from 15.8 g. p-BrC6H4Br, 4.9 g. Mg, and 100 ml. THF), the whole refluxed 2 hrs. and concentrated to dryness, the residue extracted with C6H6, the C6H6 exts. concentrated to dryness, the residue extracted with petr. ether, the petr. ether exts. concentrated to a small volume, the solid dissolved in Et2O, and the Et2O solution washed successively with 4N NaOH and 4N HCl to give 33% p-ClMe2GeC6H4GeMe2Cl (V), m. 97-102°. To 3.68 g. Na sand in 35 ml. dry PhMe was added dropwise 6.13 g. Me3GeCl and 6.52 g. IV in 75 ml. PhMe (the reaction was started by heat), the whole refluxed 11 hrs. and centrifuged, and the supernatant concentrated to give 4.9 g. Me2Ge(C6H4GeMe3)2, m. 94-6°; similarly were prepared 60% (p-Me3GeC6H4GeMe2) + C6H4 m. 105-7°, and 41% Me3Ge(C6H4GeMe2-p)3Me, m. 137-9°. Equimolar amts. of III and IV refluxed 72 hrs. with Na sand, the mixture centrifuged, the supernatant concentrated, the residue stirred with C6H6, the mixture centrifuged again, and the C6H6 solution concentrated to a small volume and poured into MeOH gave 37% (-p-Me2GeC6H4)n, (n≈ 12), m. 145-75°; the residues from the centrifugation treated with aqueous alc. and the mixture dried, continuously extracted with PhMe, and processed as above gave 4% (-p-Me2GeC6H4)n, m. 165-90°. Similarly was obtained (-p-GePh2C6H4GeMe2C6H4-)n, m. 110-30°. By the above procedure, IVa and Ph3GeBr in THF gave 46% p-Ph3GeC6H4GePh3, m. 349-50°, 41% p-Ph3SnC6H4SnPh3, m. 313-15°, and 43% p-Ph3PbC6H4PbPh3, m. 290-2°. I and Me3SnCl in THF gave 59% Me3SnC6H4Cl-p (VI), b22 122-6°, n20D 1.5516; VI and Me3SnCl gave 40% p-Me3SnC6H4SnMe3, m. 123-5°. The infrared spectra of these compds. were discussed. IT 18856-08-1, Silane, p-phenylenebis[triphenyl-

(spectrum of)

18856-08-1 HCAPLUS RN

CN Silane, 1,4-phenylenebis[triphenyl- (9CI) (CA INDEX NAME)

L22 ANSWER 9 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN Document No. 59:82319 Original Reference No. 59:15298h,15299a-c Addition and substitution reactions with triorganosilanes. Fischer, E.; Schott, G.; Petrow, A. D. (Univ., Moscow). Journal fuer Praktische Chemie (Leipzig), 21(3-4), 149-62 (Unavailable) 1968. CODEN: JPCEAO. ISSN: 0021-8383. AB SiHCl3 in ether was added to p-BrC6H4MgBr in ether, and the mixture heated to 160° over 6 hrs., treated with dilute H2SO4, and extracted with ether to give 17% tris(p-bromophenyl)silane (I), m. 106° (petr. ether). Tris(p-bromophenyl)bromosilane, m. 144-6° (petr. ether), was prepared by treating 1 mole I with 1 mole Br in 50 moles CCl4. To 3.0 g. tritolylsilane and 2.5 g. allyl bromide (II) was added 75 mg. AlCl3, and the mixture kept 6-8 hrs. at 80°, and concentrated to give 90% tritolylbromosilane, m. 127° (petr. ether). Similarly prepared R3SiBr were (R, % yield, and m.p. or b.p. given): Am, 60, b3 156°; p-ClC6H4, 90, m. 122°; p-FC6H4, 87, m. 117°. A mixture of Et3SiH and II was kept 15 hrs. at 50° under ultra-violet light. Fractionation of the products gave 24% Et3Si(CH2)3Br, b2 96°. Similarly prepared R3Si(CH2)3Br were (R, % yield, and m.p. or b.p. given): Pr, 32, b2 114°; Ph (III), 42, m. 104°. III (5.7 g.) heated at 100-200° in the presence of 0.1 g. AlCl3 gave Ph3SiCH2CH:CH2 or Ph3SiCH:CHMe, m. 78-83°. High temperature reaction of Ph3SiH and CH2: CHCH2Cl at 630° yielded 14% Ph3SiCH2CH:CH2, m. 89°. Similarly was prepared (p-ClC6H4)3SiCH2CH: CH2 (IV), 40%, m. 112°. Heating IV and CH2:CHCl at 600° yielded 36% (p-ClC6H4)3SiCH:CH2, m. 95°. IV and PhCl heated at 630° gave (p-ClC6H4)3SiCl, (p-ClC6H4)3SiPh, and (p-ClC6H4)2PhSiC6H4SiPh(C6H4Cl-p)2 (V), m. 258-62°. Similarly, IV and p-dichlorobenzene gave 20% (p-ClC6H4)3SiC6H4Si(C6H4Cl-p)3 (VI), m. 263-9°. V was obtained in 34% yield by treating 1,4-bis(phenyldichlorosily1)benzene and p-bromochlorobenzene with Na in boiling PhMe. Similarly were prepared 1,4-R3SiC6H4SiR3 (R, % yield, and m.p. given): p-ClC6H4, 32, 268-70°; Ph, 64, 314-16°; p-diphenyl, 22, 450°.

RN 18839-27-5 HCAPLUS

CN Silane, 1,1'-p-phenylenebis[tri-4-biphenylyl- (8CI) (CA INDEX NAME)

RN 18848-11-8 HCAPLUS

CN Silane, p-phenylenebis[bis(p-chlorophenyl)phenyl- (7CI, 8CI) (CA INDEX NAME)

RN 18856-08-1 HCAPLUS

CN Silane, 1,4-phenylenebis[triphenyl- (9CI) (CA INDEX NAME)

RN 18985-56-3 HCAPLUS

CN Silane, p-phenylenebis[tris(p-chlorophenyl)- (6CI, 7CI, 8CI) (CA INDEX NAME)

CC 39 (Organometallic and Organometalloidal Compounds) IT 850-60-2, Silane, bromotris(p-fluorophenyl)-17898-29-2, Silane, (3-bromopropyl)triethyl-17907-88-9, Silane, bromotripentyl-18105-60-7, Silane, (3-bromopropyl) tripropyl- 18145-72-7, Silane, trichloro(4,4,4-trinitrobutyl)-18147-78-9, Silane, trichloro(4,4-dinitrobutyl) - 18163-43-4, Silane, dichloro(4,4-dinitrobutyl)methyl- 18243-61-3, Silane, dichloromethyl (4,4,4-trinitrobutyl) -18373-69-8, Silane, tris(p-bromophenyl) - 18557-72-7, Silane, bromotris(p-chlorophenyl) - 18557-75-0, Silane, bromotris(p-bromophenyl) - 18557-76-1, Silane, chlorotris(p-chlorophenyl)-18676-73-8, Silane, 18733-89-6, Silane, tris(p-chlorophenyl)vinyltris(p-chlorophenyl)phenyl-18750-94-2, Silane, allyltri-p-tolyl-18752-22-2, Silane, 18752-21-1, Silane, allyltriphenyltriphenylpropenyl- 18752-28-8, Silane, (3-bromopropyl)triphenyl-18772-41-3, Silane, allyltris(p-chlorophenyl)-18839-27-5, Silane, p-phenylenebis[tris(4-biphenylyl)-18848-11-8, Silane, p-phenylenebis[bis(p-chlorophenyl)phenyl-18856-08-1 , Silane, p-phenylenebis[triphenyl-18985-56-3, Silane, p-phenylenebis(tris(p-chlorophenyl) -100087-61-4, Silane, bromotritoly1-(preparation of)

L22 ANSWER 10 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

1963:40116 Document No. 58:40116 Original Reference No.
58:6853g-h,6854a-c Reaction of alkenyl and aryl halides with
triarylsilanes at high temperatures. Petrov, A. D.; Fisher, E.
Zhurnal Obshchei Khimii, 32, 698-704 (Unavailable) 1962. CODEN:
ZOKHA4. ISSN: 0044-460X.

AB cf. CA 53, 1120c. p-BrC6H4MgBr, prepared in Et2O at -10° 6-8 hrs., was treated at -5° with HSiCl3 and the mixture, after 12 hrs. at room temperature and 6 hrs. at 160°, gave 17% (p-BrC6H4)3SiH, m. 104° . Similarly was prepared (m-MeC6H4)3SiH, m. 58° , and (p-FC6H4)3SiH, m. 47° . Passage of Ph3SiH with CH2: CHCH2Cl through a quartz tube at 600° (optimum temperature) gave some Ph3SiCl and 8.5% Ph3SiCH2CH:CH2, m. 89°; CH2:CHCH2Br in this reaction gave a 5% yield, along with 24% Ph3SiBr. (p-ClC6H4)3SiH and CH2:CHCH2Cl, best at 580°, gave 42% (p-ClC6H4)3SiCH2CH:CH2, m. 112°, as the sole product, although some 6% Ar3SiCl was detected by titration. (m-MeC6H4)3SiH and CH2:CHCH2Cl at 580° gave 32% (m-MeC6H4)3SiCl, m. 116-17°, and 5% (m-MeC6H4)3SiCH2CH:CH2, m. 114°. Ph3SiH and CH2:CHCH2Br gave the best yield (24%) of Ph3SiBr at 570°, while the best yield of Ph3SiCH2CH:CH2 (7%) was reached at 500°. Pure Ph3SiBr m. 114°; pure Ph3SiCH2CH: CH2 m. 87-9°. (p-ClC6H4)3SiH and CH2: CHCH2Br at 570° gave 10% (p-ClC6H4) 3SiBr, m.

122-3°, and 12% (p-ClC6H4)3SiCH2CH:CH2, m. 112°. (p-MeC6H4)3SiH and CH2:CHCH2Br at 570° gave 61% (p-MeC6H4)3SiCH2CH:CH2, m. 127°, and 3.5% (p-MeC6H4)3SiCH2CH:CH2. Ph3SiH and CH2:CHCl at 600° gave 18% Ph3SiCl and 8% Ph3SiCH:CH2, m. 58° (Henry and Noltes, CA 54, 8282f). (p-MeC6H4)3SiH and CH2:CHCl at 600° gave 32% (p-MeC6H4)3SiCl, m. 116°, and 1% (p-MeC6H4)3SiCH:CH2. (p-ClC6H4)3SiH and CH2:CHCl gave at 600° 8% (p-ClC6H4)3SiCl and 36% (p-ClC6H4)3SiCH:CH2 m. 90°. Similar reactions with CH2:CHBr gave 38-40% (p-MeC6H4)3SiBr, m. 127°, 14% Ph3SiBr, m. 119°, and 9% (p-ClC6H4)3SiBr, m. 122°, resp., while the best yield of triarylvinylsilane was 16% (p-ClC6H4)3SiCH2CH:CH2. Yield vs. temperature curves were shown. In view of enhanced reactivity of Si in arylsilanes with Cl in the ring, the following condensations were studied. PhCl and (MeC6H4)3SiH, best at 630°, gave only 2% (MeC6H4)3SiPh, along with 42% (MeC6H4)3SiCl. Ph2SiH and PhCl gave 6% Ph4Si, m. 233°, and 32% Ph3SiCl. PhCl and (p-ClC6H4)3SiH gave 8% (p-ClC6H4)3SiPh, m. 154°, and 14% (p-ClC6H4)3SiCl, as well as a polymeric product C42H30Cl4, m. 258-62°, which was probably the result of continued condensation such as C6H4(SiPhAr2)2. PhF and Ph3SiH similarly gave 4% Ph4Si and 18% Ph3SiF, m. 63°. Reaction of p-C6H4Cl2 with (p-ClC6H4)3SiH gave 12% (p-ClC6H4)3SiCl, m. 110-12°, 17% (p-ClC6H4)4Si, m. 180°, and 20% 6H4[Si(6H4Cl-p)3]2, m. 263-9°. These results indicated that the X3Si groups representing the silanes employed in this study, may be arranged in the order of electronegativity between HSiCl3 (which gave the best yields of condensation products) and Et3SiH (which did not form any condensation products). Since the electronegativities of the triarylsilanes used in this work were rather closely grouped, the large yield differences among the products of reaction could be attributed to other factors such as electronic shift from Si to Cl with reduced ionization of the Si-H bond 18985-56-3, Silane, p-phenylenebis[tris(p-chlorophenyl)-

IT (preparation of)

RN 18985-56-3 HCAPLUS

CN Silane, p-phenylenebis[tris(p-chlorophenyl)- (6CI, 7CI, 8CI) INDEX NAME)

$$\begin{array}{c} Cl \\ Cl \\ Si \\ Cl \\ \end{array}$$

39 (Organometallic and Organometalloidal Compounds) IT 379-50-0, Silane, fluorotriphenyl- 1048-08-4, Silane, tetraphenyl-1691-36-7, Silane, tris(p-fluorophenyl)-18373-69-8, Silane, s(p-bromophenyl) - 18557-72-7, Silane, bromotris(p-chlorophenyl) - 18557-76-1, Silane, chlorotris(p-chlorophenyl) - 18666-68-7, tris(p-bromophenyl)-Silane, triphenylvinyl- 18676-73-8, Silane, tris(pchlorophenyl) vinyl- 18733-81-8, Silane, tetrakis (p-chlorophenyl) -18733-89-6, Silane, tris(p-chlorophenyl)phenyl-18740-66-4,

Silane, chlorotri-p-tolyl-18742-46-6, Silane, tri-p-tolylvinyl-18750-93-1, Silane, allyltri-m-tolyl- 18750-94-2, Silane, allyltri-p-tolyl- 18752-21-1, Silane, allyltriphenyl-18752-29-9, Silane, bromotri-p-tolyl- 18766-22-8, Silane, chlorotri-m-tolyl-18772-41-3, Silane, allyltris(p-chlorophenyl)-18985-56-3, Silane, p-phenylenebis[tris(p-chlorophenyl)-27663-92-9, Silane, tri-m-tolyl- 99080-50-9, Silane, phenyltritolyl-(preparation of)

L22 ANSWER 11 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN 1962:456368 Document No. 57:56368 Original Reference No. 57:11226d-f Synthesis of p-bis[phenyl bis(p-chlorophenyl)silyl], p-bis[tris(p-chlorophenyl)silyl], and p-bis(triphenylsilyl)benzenes. Petrov, A. D.; Fisher, E. (N. D. Zelinshii Inst. Org. Chem., Moscow). Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya 168-9 (Unavailable) 1962. CODEN: IASKA6. ISSN: 0002-3353. cf. CA 55, 21010f. Heating Na with p-(Cl2SiPh)2C0H4 5 hrs. at AB 100° in the presence of p-C6H4BrCl gave 34% p-[(p-ClC5H4)2SiPh]2C6H4, m. 264°, identical with that prepared by the pyrolytic route (cf. loc. cit.). Similarly, p- (Cl3Si)2C6H6 gave 32% p-[(p-Cl6C6H4)8Si]2C0H4, m. 268-70°, identical with the product of pyrolytic synthesis. Passage of p-C5H4Cl2 and PhSiHCl2 through an empty tube at 680° with 20 sec. contact time gave 20% p-(Cl2SiPh)2C6H4, m. 96°. Similarly, HSiCl3 and p-C6H4Cl2 at 700° gave from a 2:1 reactant ratio 28% p-C6H4(SiCl3)2(I), m. 78°. This and PhCl with Na gave 44% p-C6H4(SiPh3)2, m. 314-16°. Passage of (p-PhC6H4)2SiH and p-C6H4Cl2 through a hot tube gave only 34% (p-PhC6H4)3SiCl. However, p-PhC6H4Br and I with Na gave 22% p-C6H4[Si(C6H4Ph-p)3]2, did not m. 450°. Infrared spectra of the products were

recorded. 18839-27-5, Silane, p-phenylenebis[tris(4-biphenyly1)-IT 18848-11-8, Silane, p-phenylenebis[bis(p-chlorophenyl)phenyl-18856-08-1, Silane, p-phenylenebis[triphenyl-18985-56-3, Silane, p-phenylenebis[tris(p-chlorophenyl)-(preparation of) RN 18839-27-5 HCAPLUS

Silane, 1,1'-p-phenylenebis[tri-4-biphenylyl- (8CI) (CA INDEX NAME) CN

RN 18848-11-8 HCAPLUS

CN Silane, p-phenylenebis[bis(p-chlorophenyl)phenyl- (7CI, 8CI) (CA INDEX NAME)

RN 18856-08-1 HCAPLUS CN Silane, 1,4-phenylenebis[triphenyl- (9CI) (CA INDEX NAME)

RN 18985-56-3 HCAPLUS
CN Silane, p-phenylenebis[tris(p-chlorophenyl) - (6CI, 7CI, 8CI) (CAINDEX NAME)

$$\begin{array}{c} C1 \\ C1 \\ Si \\ C1 \\ \end{array}$$

CC 33 (Organometallic and Organometalloidal Compounds)

830-46-6, Silane, p-phenylenebis[trichloro- 853-16-7, Silane, p-phenylenebis[dichlorophenyl- 2925-45-3, Silane, triethoxy(trifluorovinyl)- 18816-40-5, Silane, tris(4-biphenylyl)chloro-18839-27-5, Silane, p-phenylenebis[tris(4-biphenylyl)-18848-11-8, Silane, p-phenylenebis[bis(p-chlorophenyl)phenyl-18856-08-1, Silane, p-phenylenebis[triphenyl-18985-56-3, Silane, p-phenylenebis[tris(p-chlorophenyl)- (preparation of)

L22 ANSWER 12 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN 1962:456367 Document No. 57:56367 Original Reference No. 57:11226c-d

The reduction of aromatic compounds by lithium in low-molecular weight amines. Stereochemistry of the addition of trichlorosilane to acetylenes. Factors influencing the direction of elimination in xanthate pyrolysis. Burrous, Merwyn L. (Purdue Univ., Lafayette, IN). 124 pp. Avail. Univ. Micro films (Ann Arbor, Mich.), Order No. 61-5699 From: Dissertation Abstr. 22, 4179-80 (Unavailable) 1962.

AB Unavailable

RN 18856-08-1 HCAPLUS

CN Silane, 1,4-phenylenebis[triphenyl- (9CI) (CA INDEX NAME)

L22 ANSWER 13 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

1962:449397 Document No. 57:49397 Original Reference No.

57:9871c-i,9872a-c Studies in IVth group organometallic chemistry.

IX. Synthesis of organosilicon compounds and polymers containing the p-phenylene group. Noltes, J. G.; van der Kerk, G. J. M. (Inst. Org. Chem., Utrecht, Neth.). Recueil des Travaux Chimiques des Pays-Bas, 81, 565-77 (English) 1962. CODEN: RTCPA3. ISSN:

0165-0513. cf. CA 56, 15530i. A solution of p-ClC6H4MgCl, from 162 g. p-C6H4Cl2 and 26.5 g. Mg in 300 ml. tetrahydrofuran (I), was added slowly with vigorous stirring to 150 g. Me2SiCl2 (II) in 200 ml. I (all reactions carried out under dry N), the mixture heated 2 hrs. at 50°, the solvent evaporated, and 300 ml. petr. ether added to the vigorously stirred residue. The mixture was filtered, the solvent evaporated, and the residue fractionated to give 30% p-ClC6H4SiMe2Cl (III), b18 106-9°, n20D 1.5232. p-C6H4Br2 (IV) (88 g.) in 250 ml. Et20 was added, over 5 hrs. with vigorous stirring, to 142 g. II, 27 g. Mg, a crystal of iodine, and 75 ml. Et20, the mixture refluxed 3 hrs., cooled, filtered, concentrated, again filtered, the solvent evaporated, and the residue fractionated to give 44% p-C6H4(SiMe2Cl)2 (V), m. 85-8°, b0.3 116-22°, b19 150-5°. p-ClC6H4SiMe3 (VI) (18.5 g.) in 60 ml. I was refluxed 9 hrs. with excess Mg, 18.5 g. III in 35 ml. I added dropwise, the mixture refluxed 3 hrs., then decomposed with aqueous NH4Cl, and worked up through Et2O to give 52% R' (p-C6H4SiR''2)nR''' (VII) (R' = Cl, R'' = R''' = Me, n = 2) (VIII), b0.1 129-32°, n2OD 1.5507. The Grignard reagent from 59 g. IV and 12 g. Mg in 350 ml. I was added over 3 hrs. to 157 g. Ph2SiCl2 (IX) in 125 ml. I at 50°, I evaporated, the residue dissolved in C6H6, the solution filtered, and evaporated to dryness to give a product which was refluxed 1 hr. with 1 1. EtOH. The solution, concentrated and cooled to 0°, gave 42% compound, m. 150-5°, repeated crystallization of which gave 17% p-C6H4(SiPh2OEt)2 (X), m. 158-60° (EtOH). Anhydrous HCl passed into X in Et2O precipitated p-C6H4(SiPh2Cl)2 (XI), m. 195-80 (ligroine). V (7.8 g.) in 30 ml. PhMe was stirred into 45 ml. PhMe containing 10.9 g. VI and 3.5 g. Na sand, at such a rate as to maintain reflux, the mixture refluxed 6 hrs., centrifuged, the precipitate extracted once with boiling PhMe, and the solvent removed to give 37% VII (R' = SiMe3, R'' = R''' = Me, n = 3), m. 131-3° (EtOH). Similarly were prepared (reactants, product, m.p., recrystg. solvent, and % yield given): Me3SiCl and VI (with Mg and I replacing Na and PhMe),

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p-C6H4(SiMe3)2, 94-6°, EtOH, 60; II and VI,
Me2Si(p-C6H4SiMe3)2, 78-81°, PrOH, 48; II and VIII, VII (R' =
SiMe3, R'' = R''' = Me, n = 4), 170-3°, Me2CO, 53; V and VIII, VII (R' = SiMe3, R'' = R''' = Me, n = 5) (XII),
187-91°, PhMe, 47; V and p-ClC6H4SiPh3 (XIII), VII (R' = SiPh3, R'' = Me, R''' = p-C6H4SiPh3, n = 2), 220-2°, Me2NCHO, 48. Ph3SiBr (8.47 g.), 9.27 g. XIII, and 1.2 g. Na sand in 75 ml.
PhMe was refluxed 10 hrs. after spontaneous heating ceased. The
cooled mixture was centrifuged, the precipitate washed with aqueous EtOH, and
continuously extracted with Me2NCHO. The extract deposited 33%
p-C6H4(SiPh3)2, m. 337-41°. Similarly Ph2SiCl2 and XIII gave 45% Ph2Si(p-C6H4SiPh3)2, m. 3658° (xylene). A p-chlorophenylsilane in PhMe was added dropwise to a vigorously
stirred mixture of 1 molar equivalent of a chlorosilane and excess Na sand
in PhMe, the mixture refluxed 4-6 days, then centrifuged. The
supernatant liquor was poured into MeOH, the precipitate redissolved in
PhMe, and MeOH added portionwise to precipitate fraction A. The precipitate from
centrifugation was washed with aqueous EtOH, dried, and continuously
extracted with PhMe to give a solution from which MeOH precipitated fraction B.
Thus were prepared (p-chlorophenyl) silane, chlorosilane, fraction
containing polymer, poly-p-phenylenesilane, m.p., % yield, and
number-average mol. weight given): Me2Si(p-C6H4Cl)2 (XIV), II, B,
(SiMe2C6H4)28 (XV), 200-25°, 15, 3800; XIV, II, A, (SiMe2C6H4)13, 155-210°, 54, 1800: III, III, B, (SiMe2C6H4)16, 190-210°, 17, 2100; III, III, A,
(SiMe2C6H4)13 (XVI), 170-85°, 40, 1800; Ph2Si(p-C6H4Cl)2
(XVII), II, not precipitated by MeOH, (SiMe2-C6H4SiPh2C6H4)6 (XVIII),
155-70°, 76, 2400; XVII, V, B, (SiMe2C6H4SiMe2C6H4SiPh2C6H4)6
(XIX), 190-210°, 14, 2900; XVII, V, A, (SiMe2C6H4SiMe2C6H4SiPh2C6H4)5, 175-95°, 34, 2800; XIV, XI,
B, (SiMe2C6H4SiPh2C6H4SiPh2C6H4)4 (XX), 215-45°, 18, 2600;
XIV, XI, A, (SiMe2C6H4SiPh2C6H4SiPh2C6H4)n, 135-55°, 22, --;
XVII, XI, residue insol. in PhMe, (SiPh2C6H4), (XXI), >360°,
52, --; XVII, XI, B, (SiPh2C6H4)8 (XXII), 235-60°, 12, 2100.
The low mol. wts. of the polymers are due to chain-termination by
the solvent. Thermogravimetric data are given for XII, XV, XVI,
XVIII-XXII. 17 references.
18827-38-8, Silane, diphenylbis[p-(triphenylsilyl)phenyl]-
18856-08-1, Silane, p-phenylenebis[triphenyl-
    (preparation of)
18827-38-8 HCAPLUS
Silane, diphenylbis[p-(triphenylsilyl)phenyl] - (7CI, 8CI)
                                                                        (CA INDEX
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RN 18856-08-1 HCAPLUS CN Silane, 1,4-phenylenebis[triphenyl- (9CI) (CA INDEX NAME)

IT

RN CN

CC 33 (Organometallic and Organometalloidal Compounds)
IT 825-92-3, Silane, chloro(p-chlorophenyl)dimethyl- 1078-97-3,

Silane, p-phenylenebis[chlorodimethyl- 10466-89-4, Silane, p-phenylenebis[chlorodiphenyl- 13183-70-5, Silane, p-phenylenebis[trimethyl- 14814-13-2, Silane, p-phenylenebis[ethoxydiphenyl- 18057-52-8, Silane, 1-(p-chlorophenyl)-1,1,1',1',1'-pentamethyl-1,1'-p-phenylenebis-18589-10-1, Silane, dimethylbis[p-(trimethylsilyl)phenyl]-18817-60-2, Silane, bis[p-[dimethyl[p-(trimethylsilyl)phenyl]silyl]phenyl]dimethyl- 18825-51-9, Silane, p-phenylenebis[dimethyl[p-(triphenylsilyl)phenyl]-18827-38-8, Silane, diphenylbis[p-(triphenylsilyl)phenyl]- 18828-76-7, Silane, p-phenylenebis[[p-[dimethyl[p-(trimethylsilyl)phenyl]silyl]phenyl]dimethyl- 18848-18-5, Silane, p-phenylenebis[dimethyl[p-(trimethylsilyl)phenyl]-18856-08-1, Silane, p-phenylenebis[triphenyl-(preparation of)

L22 ANSWER 14 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

1961:111860 Document No. 55:111860 Original Reference No. 55:21010f-h
High temperature reaction of triarylsilanes with allyl chloride, and
chloro- and p-dichlorobenzenes. Fisher, E.; Petrov, A. D. (D. I.
Mendeleev Chem.-Technol. Inst., Moscow). Doklady Akademii Nauk
SSSR, 138, 136-8 (Unavailable) 1961. CODEN: DANKAS. ISSN:
0002-3264.

cf. Ponomarenko and Egorov, CA 54, 22005a. Heating CH2:CHCH2Cl with (p-ClC6H4)3SiH (best at 580°) gave 42% (p-ClC6H4)3SiCH2CH:CH2, m. 112°, and 6% (p-ClC6H4)3SiCl. Similarly, at 580° (p-MeC6H4)3SiH gave 32% (p-MeC6H4)3SiCl (I), m. 116-17°, and 5% (p-MeC6H4)3SiCH2CH:CH2, m. 114°. (p-MeC6H4)3SiH and PhCl at 630° gave 2% (p-MeC6H4)3SiPh and 42% I. PhCl and (p-ClC6H4)3SiH gave 14% (p-ClC6H4)3SiCl and 19% (p-ClC6H4)3SiPh. The last reaction also gave an unidentified substance, m. 258-62°, Si2Cl4C42H20, possibly a condensation product. Similarly, (p-ClC6H4)3SiH and p-C6H4Cl2 gave 12% (p-ClC6H4)3SiCl and 17% (p-ClC6H4)4Si, m. 180°; much HCl and polymeric product, m. 263-9°, was isolated; the polymer appeared to be mainly bis[tri-(pchlorophenyl) silyl] benzene. IT 18985-56-3, Silane, p-phenylenebis[tris(p-chlorophenyl)-

(preparation of)
RN 18985-56-3 HCAPLUS

CN Silane, p-phenylenebis[tris(p-chlorophenyl) - (6CI, 7CI, 8CI) (CA INDEX NAME)

CC 10E (Organic Chemistry: Benzene Derivatives)
IT 18557-76-1, Silane, chlorotris(p-chlorophenyl) - 18733-81-8,
Silane, tetrakis(p-chlorophenyl) - 18733-89-6, Silane,
tris(p-chlorophenyl)phenyl - 18740-66-4, Silane, chlorotri-p-tolyl-

18750-94-2, Silane, allyltri-p-tolyl-18772-41-3, Silane, allyltris(p-chlorophenyl) - 18870-40-1, Silane, phenyltri-p-tolyl-18985-56-3, Silane, p-phenylenebis[tris(p-chlorophenyl)-(preparation of)

L22 ANSWER 15 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN 1961:43307 Document No. 55:43307 Original Reference No. 55:8424g-i,8425a-h o-Phenylene silicon derivatives. Dihydrosilanthrene and related compounds. Gilman, Henry; Zuech, Ernest A. (Iowa State Univ., Ames). Journal of the American Chemical Society, 82, 3605-8 (Unavailable) 1960. CODEN: JACSAT. ISSN: 0002-7863.

GΙ

For diagram(s), see printed CA Issue. AB cf. CA 54, 9947i. During a successful effort to prepare I (5,5,10,10-tetrasubstituted-5,10-dihydrosilanthrenes), o-C6H4Li2 (II) was treated with Ph2SiH2 (III), MePh2SiCl (IV), Ph2SiCl2 (V), (PhCH2)2SiCl2 (VI), o-C6H4(SiHPh2)2 (VII), and Ph3SiCl (VIII). The reactions of VII with MeLi and PhLi were also investigated. Acid titration of Et2O solns. of II that had been filtered through glass wool indicated over 100% base present, but acceptable values were obtained if solns. were first filtered through a sintered glass filter. A solution of II, prepared (Wittig and Bickelhaupt, CA 52, 18307b) by shaking 8.28 g. o-phenylene-mercury (IX) and 6 g. Li wire in 100 ml. dry Et2O 4 days was added during 30 min. to 5.52 g. III in 50 ml. Et20 in an ice-bath, the mixture stirred 24 hrs. at room temperature, hydrolyzed with 100 ml. 5% HCl, Et2O added, the mixture filtered, and the solid crystallized to give 1.64 g. VII, m. 174-6° (EtOAc); from the hydrolysis filtrate was isolated 0.77 g. addnl. VII, m. 174-6° (total yield, 36%); anal. sample m. 174.5-6.0°. When a solution of II (from 10 g. IX and 7 g. Li) was added to 14.7 g. III in 100 ml. Et20 and after 16 hrs. the mixture hydrolyzed with dilute H2SO4, 23% VII was obtained. Treatment of 0.06 mole III with II in a 0.024 mole solution that had been filtered through a sintered glass filter yielded 38% VII. II (0.023 mole) filtered through a glass filter, added to 0.023 mole III in Et20, the mixture stirred 17 hrs., 50 ml. PhMe added, Et20 removed by distillation, the suspension refluxed 3 hrs. (Color Test I neg.), hydrolyzed, and the Et2O layer evaporated gave an oil, which upon chromatography on Al2O3 yielded 0.1 g. Ph3SiH, 2.7% Ph4Si, m. 234-7° (EtOAc), 31% VII, m. 175-7° (EtOAc), and 9.1% o-Ph3SiC6H4(SiHPh2) (X), m. 214-17° (EtOAc). A solution of II, prepared from 10 g. IX, was added to 17.4 g. IV in Et20, refluxed 18 hrs. (Color Test I pos.), 80 ml. PhMe added, Et20 removed by distillation, the mixture refluxed 24 hrs., and hydrolyzed to give an oil, which when extracted with petr. ether and recrystd. from petr. ether yielded 29% (MePh2Si)2 (mixed m.p. and infrared comparison); concentration of the petr. ether extract and recrystn. of the precipitate gave 7.7% o-C6H4(SiPh2Me)2 (XI), m. 173-4° (petr. ether). MeLi (0.007 mole) added to 1 g. VII in 50 ml. Et20, the mixture refluxed 18 hrs., treated with 0.003 mole addnl. MeLi, 40 ml. PhMe added, Et20 removed by distillation, and the mixture refluxed 1 hr. gave 0.82 g. solid, m. 125-52°, from which 17% XI, m. 171-3°, was obtained by 6 recrystns. from petr. ether (purification was difficult owing to the presence of SiH-containing compds.). II (0.028 mole) in Et2O was added to 7.1 g. V in 25 ml. Et2O, the mixture stirred 18 hrs., 50 ml. PhMe added, Et20 removed by distillation, the mixture refluxed 6 hrs. (Color Test I neg.), hydrolyzed with dilute H2SO4, the H2O layer extracted with Et20, the combined Et20 layers evaporated, and the residue chromatographed on Al2O3 to give 0.6% Ph4Si, m. 234-7° (EtOAc), and 10% I (R = Ph), m. $234-6^{\circ}$ (EtOAc), b. 540° (slight decomposition). II, prepared from 4.15 g. IX, was added to 4.42 g. VII in 100 ml. dry PhMe, Et20 removed by distillation, the mixture refluxed 5 hrs., hydrolyzed with ice and dilute H2SO4, Et20 added, and the mixture worked up as usual to give an oil, which upon crystallization from EtOAc yielded 15% X, m. 214-16°. From 0.012 mole II and 0.012 mole VII was obtained 23% X plus 38% recovered

VII. A solution of 7.3 g. VI in 75 ml. Et20 in an ice-bath was treated with 0.026 mole II in Et20, the mixture stirred 16 hrs. at room temperature (Color Test I pos.), 30 ml. PhMe added, Et20 removed by distillation, the mixture refluxed 4 hrs. (Color Test I neg.), and hydrolyzed to give 2.8% I (R = PhCH2), m. 174.5-6.0 (10:1 petr. ether-C6H6), b. 510° (decomposition). PhLi (0.015 mole) in Et20 added to 2.21 g. VII in 100 ml. Et20, the mixture refluxed 24 hrs. and hydrolyzed yielded 24% crude X and 31% o-C6H4(SiPh3)2 (XII), m. 257.5-9.0° (EtOAc). X (1.35 g.) in 50 ml. dry PhMe was treated with 0.01 mole PhLi in Et2O, the Et2O removed by distillation, the mixture refluxed 16 hrs., an addnl. 0.003 mole PhLi added, the mixture refluxed 8 hrs. and hydrolyzed, to give 73% XII, m. 256-9° (EtOAc). A solution of 8.23 g. VIII in 100 ml. Et20 was treated with 0.014 mole II in Et20, 75 ml. PhMe added, the Et20 distilled, and the mixture refluxed 24 hrs. to give 14% (Ph3)20 and 21% Ph3SiOH. Attempts to make mol. models of XI and XII indicated considerable strain.

IT 18920-15-5, Silane, o-phenylenebis[triphenyl-

(preparation of)
RN 18920-15-5 HCAPLUS

CN Silane, o-phenylenebis[triphenyl- (6CI, 8CI) (CA INDEX NAME)

CC 10G (Organic Chemistry: Heterocyclic Compounds)

IT 789-25-3, Silane, triphenyl- 791-31-1, Silanol, triphenyl1048-08-4, Silane, tetraphenyl- 1172-76-5, Disilane,
1,2-dimethyl-1,1,2,2-tetraphenyl- 1829-40-9, Disiloxane,
hexaphenyl- 18815-90-2, Silane, pentaphenyl-o-phenylenebis18817-06-6, Silanthrene, 5,10-dihydro-5,5,10,10-tetraphenyl18839-04-8, Silane, o-phenylenebis[methyldiphenyl- 18845-58-4
Silanthrene, 5,5,10,10-tetrabenzyl-5,10-dihydro- 18881-83-9,
Silane, o-phenylenebis[diphenyl-18920-15-5, Silane,
o-phenylenebis[triphenyl(preparation of)

L22 ANSWER 16 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

1959:56212 Document No. 53:56212 Original Reference No.
53:10102g-i,10103a-i,10104a-c Cleavage of diphenyl sulfone and diphenyl sulfide by triphenylsilyllithium. Wittenberg, Dietmar; Wu, T. C.; Gilman, Henry (Iowa State Coll., Ames). Journal of Organic Chemistry, 23, 1898-1903 (Unavailable) 1958. CODEN: JOCEAH. ISSN: 0022-3263.

AR Ph3SiLi (I) was found to cleave Ph2SO2 (II) with the formation of PhLi (III) and triphenyl(phenylsulfonyl) silane (IV), which in a 2nd step interact to give Ph4Si (V) and Li benzenesulfinate (VI). In addition, a variety of other products was obtained when excess I was used. The reaction of I with Ph2S (VII) gave, in addition to Ph6Si2 (VIII), III and Li thiophenolate (IX) as the cleavage products. (0.058 mole) in tetrahydrofuran added to 8.25 g. II accompanied by external cooling, and after hydrolysis and addition of some ether 4.4 g. V, m. 232-4°, which when dissolved in C6H6 left 0.13 g. insol. material, which was shown to be impure mphenylenebis(triphenylsilane) (IXa), m. 345-9°. The layers of the filtrate separated, the organic layer washed, dried, and evaporated gave $2\ g.\ V.$ When C6H6 was added to the concd, mother liquor $0.18\ g.$ precipitate formed, m. 280-320°, which was not further identified. Addition of ligroine gave 2.9 g. triphenylsilanol (X), m. 151-3°, and a small amount of hexaphenyldisiloxane (Xa), m. 225-8°. The combined aqueous layers gave after acidification an

orange precipitate with FeCl3 solution which was insol. in dilute HCl, which indicated the presence of benzenesulfinic acid which came from VI. A sample of the aqueous solution refluxed 0.5 hr. with an equal volume of alc. HgCl2 gave a small amount of PhHgCl, m. 151-2°. Second experiment: I (0.076 mole) in tetrahydrofuran treated 72 hrs. with 8.25 g. II and hydrolyzed gave 4.85 g. IXa, identical with a specimen obtained from m-phenylenebis(trichlorosilane) and III. The C6H6 solution gave on concentration a small amount of impure VIII, m. 856-63°, and further concentration gave 3.5 g. V. The layers of the 1st filtrate separated, some Et20 added, the organic layer washed, dried, and distilled gave 1.1 g. Xa. From the filtrate 1.4 g. X was obtained. The aqueous layer of the run showed the same properties as in the 1st experiment The presence of benzenesulfinic acid (XI) was estimated by reactions with FeCl3 and HgCl2. Third experiment: I (0.048 mole) in tetrahydrofuran added during 15 min. at room temperature to 5.2 g. II, stirred 1 hr., poured on Dry Ice, extracted with Et2O, and worked up gave 1.4 g. IXa and 0.25 g. VIII. The 2 layers of the first filtrate separated, the organic layer extracted with dilute NaOH, then with H2O, dried, the solvents distilled and the residue chromatographed gave 0.45 g. V and 3.1% Xa. The ligroine-alc, filtrate concentrated and treated with ligroine gave 3.95 g. X and no crystalline material was obtained from the mother liquor but the infrared spectrum indicated the presence of Ph3SiH with further evidence being the evolution of H gas on treatment with KOH The alkaline aqueous layer refluxed a few min., and the solid removed gave 2.1 g. 4-(triphenylsilyl)benzoic acid, m. 213-14° (AcOH and cyclohexane). The alkaline aqueous filtrate acidified gave 1.93 g. crude product indicating the presence of XI. The crude acidic material extracted with ligroine gave 0.5 g. BzOH, m. 121-2° (H2O). Fourth experiment: I (0.0396 mole) in tetrahydrofuran added slowly at -30 to -40° to 4.31 g. II, stirred at this temperature 5 hrs., kept overnight at -70°, carbonated, extracted with Et20, then with dilute NaOH, the organic layer dried, distilled, and the oily residue chromatographed on Al2O3 gave 0.2 g. Ph3SiH and 0.25 g. V. Final elution with Me2CO gave 6.1 g. The alkaline aqueous layer acidified and extracted with Et2O gave some XI and 2.1 g. BzOH. Fifth experiment: I (0.069 mole) in tetrahydrofuran added to 5 g. II, the mixture stirred 48 hrs. at room temperature, hydrolyzed, extracted with Et2O, and filtered to give 7.1 g. crude IXa and 1.5 g. V. The filtrate layers separated, the organic layer washed, dried, and distilled gave 4.2 g. crude material which was chromatographed to give 1.3 g. V, 2.75 g. Xa; no pure crystalline product was isolated from the 1st ligroinealc.-filtrate. Acidification of the alkaline aqueous layer caused evolution of H2S and gave an orange precipitate with FeCl3 indicative of XI. Refluxing the solution a few min. gave the characteristic odor of thiophenol. I (0.0244 mole) in tetrahydrofuran stirred 2 hrs. at room temperature with 6 g. di-p-tolyl sulfone, the mixture carbonated as usual, H2O and Et2O added, 0.2 g. VIII collected, the filtrate layers separated, the organic layer extracted with dilute NaOH, and after removal of the solvent the oily residue chromatographed on Al2O3 gave 3.25. g. Ph3SiH, 0.3 g. di-p-tolyl sulfone, m. 156-8°, 1.55 g. X, and finally 0.8 g. unidentified compound, decomposed without m. about 370°. Acidification of the alkaline aqueous layer gave a precipitate with FeCl3 indicative of a sulfinic acid; the solution extracted with Et2O, the organic layer dried, and distilled gave 0.55 g. p-toluic acid, m. 178-80° (H2O). VIII (0.01 mole) cleaved with excess Na-K in Et20 gave a Ph3SiK (XII) suspension. This suspension left 24 hrs. at room temperature with 4.4 g. II in 70 ml. C6H6, the mixture hydrolyzed, filtered, and recrystd. gave 1.3 g. VIII. The organic solution dried and distilled gave 1.2 g. V. I (0.015 mole) in 20 ml. tetrahydrofuran stirred 5 hrs. at room temperature with 5 g. V, then carbonated, treated with H2O and Et2O, and separated gave $4.7~\rm g.~V.$ The organic layer gave 4g. crude X. III in tetrahydrofuran was obtained in 96% yield. III (0.0246 mole) and 0.0246 mole I in tetrahydrofuran stirred 6 hrs. at -30 to -40°, kept overnight at -70° carbonated, H20 and Et2O added, and the solvent evaporated gave 2.3 g. crude BzOH. No

H2O insol. acidic fraction was found. The organic layer gave 0.2 q. V and 0.31 g. mixture of Xa and V. The alc. filtrate gave 3.8 g. X. a 2nd run using the same amts. of reagents the mixture stirred 1.5 hrs. at room temperature, and then carbonated and separated as above gave 1.6 g. crude BzOH, 0.9 g. V together with 0.55 g. mixed V and Xa, and 3.8 g. X. I (0.036 mole) in tetrahydrofuran added at -50° to 6.2 g. PhSO2Cl, the mixture warmed to room temperature, and filtered gave 6.2 g. VIII. The filtrate gave 2.65 g. putative mixture of LiCl and VI. The aqueous solution gave an orange precipitate with FeCl3. The ligroine filtrate gave 0.21 g. Xa. No other crystalline products were isolated from the mother liquors. I (0.018 mole) in tetrahydrofuran was added to 3.72 g. VII; heat was evolved and the color changed to brown; after 10 min. the color test was still strongly pos. and the mixture carbonated gave 2.95 g. VIII. The filtrate layers on separation gave 0.35 g. X and 1.2 g. VII from the organic layer. The aqueous layer on acidification gave the odor of thiophenol showing the previous presence of IX. Et2O extraction gave 0.32 g. BzOH. When in a 2nd experiment I was allowed to react with VII 5 hrs. at -30°, the workup by carbonation gave only traces of acidic material and traces of VIII. VII and X were recovered in high yields. XII in Et2O stirred 24 hrs. with 0.02 mole VII, the mixture hydrolyzed, the Et2O solution dried and evaporated gave a residue indicative of thiophenol. The crude residue yielded 3.5 g. X and 0.2 g. V. Diphenyl sulfoxide (4 g.) in 50 ml. Et2O stirred 45 min. with a XII suspension in Et2O, the mixture hydrolyzed, and 0.6 g. VIII collected, the Et2O solution evaporated and the residue crystallized gave 1.1 g. IXa and 0.9 g. V. Dibenzothiophene under the same conditions was not attacked by I.

IT 18920-16-6, Silane, m-phenylenebis[triphenyl-

(preparation of) RN

18920-16-6 HCAPLUS

CN Silane, 1,3-phenylenebis[triphenyl- (9CI) (CA INDEX NAME)

CC 10E (Organic Chemistry: Benzene Derivatives) IT 100-56-1, Mercury, phenyl-, chloride 108-98-5, Benzenethiol 618-41-7, Benzenesulfinic acid 789-25-3, Silane, triphenyl-791-31-1, Silanol, triphenyl- 1048-08-4, Silane, tetraphenyl-1450-23-3, Disilane, hexaphenyl- 1829-40-9, Disiloxane, hexaphenyl- 16883-74-2, Benzenesulfinic acid, lithium salt 18738-01-7, Silane, triphenyl (phenylsulfonyl) - 18821-83-5, Benzoic acid, p-(triphenylsilyl)-18920-16-6, Silane, m-phenylenebis[triphenyl-(preparation of)

=> d 123 1-5 cbib abs hitstr hitind

L23 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN 2002:831328 Document No. 138:303947 Ir and Rh complex-catalyzed intramolecular alkyne-alkyne couplings with carbon monoxide and isocyanides. Shibata, Takanori; Yamashita, Koji; Katayama, Emi; Takagi, Kentaro (Faculty of Science, Department of Chemistry, Okayama University, Tsushima, Okayama, 700-8530, Japan). Tetrahedron, 58(43), 8661-8667 (English) 2002. CODEN: TETRAB. ISSN: 0040-4020. OTHER SOURCES: CASREACT 138:303947. Publisher: Elsevier Science Ltd.. AR

Intramol. [2+2+1] cycloaddn. of diynes with carbon monoxide was catalyzed by Vaska's complex (IrCl(CO)(PPh3)2) or IrCl(cod)(dppp), and cyclopentadienones were obtained in good to high yields. The first catalytic synthesis of iminocyclopentadienes was achieved by

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portionwise addns. of isocyanides to a solution of diynes and Rh
catalyst ([RhCl(cod)]2). The carbonylchlorobis(triphenylphosphine)i
ridium-catalyzed carbonylative coupling of 1,1'-(1,6-heptadiyne-1,7-
diyl)bis[benzene] (I) gave 1,1'-(1,6-heptadiyne-1,7-diyl)bis[benzene] in 79% yield. The diµ-chlorobis[(1,2,5,6-
η)-1,5-cyclooctadiene]diiridium-catalyzed coupling of I with
2-isocyano-1,3-dimethylbenzene in di-Bu ether gave
N-(5,6-dihydro-1,3-diphenyl-2(4H)-pentalenylidene)-2,6-
dimethylbenzenamine (iminocyclopentadiene) in 83% yield.
340180-13-4P, 7,9-Bis(triphenylsilyl)-8H-
Cyclopent[a] acenaphthylen-8-one
RL: SPN (Synthetic preparation); PREP (Preparation)
   (iridium and rhodium complex-catalyzed intramol. alkyne-alkyne
   couplings with carbon monoxide and isocyanides)
340180-13-4 HCAPLUS
8H-Cyclopent[a]acenaphthylen-8-one, 7,9-bis(triphenylsilyl) - (9CI)
(CA INDEX NAME)
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CC 24-4 (Alicyclic Compounds)

Section cross-reference(s): 25 IT 121573-71-5P, N-(5,6-Dihydro-1,3-diphenyl-2(4H)-pentalenylidene)-2,6dimethylbenzenamine 154353-74-9P, 3,5-Dihydro-5-oxo-4,6-diphenyl-2,2(1H)-Pentalenedicarboxylic acid diethyl ester 340180-12-3P, 4,6-Bis(triphenylsilyl)-1H-Cyclopenta[c]furan-5(3H)-one 340180-13-4P, 7,9-Bis(triphenylsilyl)-8H-Cyclopent[a]acenaphthylen-8-one 340180-16-7P, 3,5-Dihydro-5-oxo-4,6-diphenyl-2,2(1H)-Pentalenedicarboxylic acid bis(1,1dimethylethyl) ester 340180-17-8P 340180-18-9P, 4,6-Bis(4-chlorophenyl)-3,5-dihydro-5-oxo-2,2(1H)-Pentalenedicarboxylic acid bis(phenylmethyl) ester 340180-20-3P 340180-21-4P, 5,6-Dihydro-1,3-diphenyl-2(4H)-Pentalenone 340180-22-5P, 4,6-Diphenyl-1H-Cyclopenta[c]furan-5(3H)-one 340180-23-6P, 4,5-Dihydro-5-oxo-4,6-diphenyl-2,2(1H)-Pentalenedicarboxylic acid bis(phenylmethyl) ester 340180-24-7P 340180-26-9P 340180-25-8P 507990-03-6P 507990-08-1P 507990-17-2P 507990-24-1P 507990-29-6P 507990-40-1P 507990-53-6P, N-(5,6-Dihydro-1,3-diphenyl-2(4H)-pentalenylidene)-4-508020-95-9P methoxybenzenamine RL: SPN (Synthetic preparation); PREP (Preparation) (iridium and rhodium complex-catalyzed intramol. alkyne-alkyne couplings with carbon monoxide and isocyanides)

L23 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
2001:187908 Document No. 134:366615 Iridium Complex Catalyzed
Carbonylative Alkyne-Alkyne Coupling for the Synthesis of
Cyclopentadienones. Shibata, Takanori; Yamashita, Koji; Ishida,
Hiroyuki; Takagi, Kentaro (Department of Chemistry Faculty of
Science, Okayama University, Tsushima Okayama, 700-8530, Japan).
Organic Letters, 3(8), 1217-1219 (English) 2001. CODEN: ORLEF7.
ISSN: 1523-7060. OTHER SOURCES: CASREACT 134:366615. Publisher:
American Chemical Society.

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Fused cyclopentadienones I [X = 0, H2C, (EtO2C)2C, (PhCH2O2C)2C; R = Ph3Si, Ph, 4-MeOC6H4, 4-ClC6H4, 4-MeO2CC6H4] are prepared in 52-99% yields by catalytic carbonylative alkyne-alkyne coupling of the bisalkynes RC.tplbond.CCH2XCH2C.tplbond.CR II using iridium diphosphine complexes under carbon monoxide at atmospheric pressure or a partial pressure of 0.2 atmospheric Either Ir(1,5-COD) (Ph2PCH2CH2CH2PPh2)Cl2 or Ir(1,5-COD) (Ph3P)2Cl2 (Vaska's complex) are optimal catalysts for this process. E.g., stirring II [R = Ph; X = (PhCH2O2C)2C] in xylene under 1 atmospheric CO pressure at 120° in the presence of Vaska's complex for 2-7 h gives I [R = Ph; X = (PhCH2O2C)2C] in 99% yield. The crystal structure of the chloroform solvate of the iridium biphosphine Ir(1,5-COD) (Ph2PCH2CH2CH2PPh2)Cl2 [Ir(COD) (dppp)Cl•CHCl3] was determined IT 340180-13-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of fused cyclopentadienones by cyclocarbonylation of bisalkynes under a carbon monoxide atmospheric in the presence of iridium diphosphine catalysts)

RN 340180-13-4 HCAPLUS

CN 8H-Cyclopent[a]acenaphthylen-8-one, 7,9-bis(triphenylsilyl)- (9CI) (CA INDEX NAME)

Ph3Si

CC 24-7 (Alicyclic Compounds)

Section cross-reference(s): 27, 29, 75

IT 154353-74-9P 340180-12-3P**340180-13-4P** 340180-15-6P 340180-16-7P 340180-17-8P 340180-18-9P 340180-20-3P

340180-21-4P 340180-22-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of fused cyclopentadienones by cyclocarbonylation of bisalkynes under a carbon monoxide atmospheric in the presence of iridium diphosphine catalysts)

L23 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

2000:803531 Document No. 134:147326 Inter- and intramolecular carbonylative alkyne-alkyne coupling reaction mediated by cobalt carbonyl complex. Shibata, T.; Yamashita, K.; Takagi, K.; Ohta, T.; Soai, K. (Department of Chemistry, Faculty of Science, Okayama University, Tsushima, Okayama, 700-8530, Japan). Tetrahedron, 56(47), 9259-9267 (English) 2000. CODEN: TETRAB. ISSN: 0040-4020. OTHER SOURCES: CASREACT 134:147326. Publisher: Elsevier Science Ltd..

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AB Inter- and intramol. carbonylative coupling reactions between alkynes possessing diphenylallylsilyl groups mediated by dicobalt carbonyl complexes under argon atmospheric gave mono- and bicyclic cyclopentadienones in high yields. Thus, reaction of BuC.tplbond.CSiPh3 (I) and the hexacarbonyldicobalt complex of I in toluene at 120° gave 77% of a 3.5:1 mixture of cyclopentadienones II and III.

IT 212125-17-2P 212125-18-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of disilylcyclopentadienones via intermol. and intramol. cycloaddn./coupling reactions of silyl alkynes and hexacarbonyl(silyl alkyne)dicobalt complexes)

RN 212125-17-2 HCAPLUS

CN 2,4-Cyclopentadien-1-one, 3,4-dibutyl-2,5-bis(triphenylsilyl)- (9CI) (CA INDEX NAME)

CC 24-4 (Alicyclic Compounds)
 Section cross-reference(s): 29

IT 212125-14-9P 212125-15-0P 212125-16-1P212125-17-2P 212125-18-3P 212125-19-4P 212125-20²7P 212125-21-8P 212125-25-2P 212125-26-3P 212125-32-1P 212125-33-2P 212125-34-3P 212125-36-5P 324000-49-9P 324000-60-4P 324000-61-5P 324000-62-6P 324000-63-7P 324000-64-8P

324000-65-9P 324000-67-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of disilylcyclopentadienones via intermol. and intramol. cycloaddn./coupling reactions of silyl alkynes and hexacarbonyl(silyl alkyne)dicobalt complexes)

L23 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN 1998:495679 Document No. 129:202694 Direct synthesis of

cyclopentadienones by cobalt carbonyl-mediated carbonylative alkyne-alkyne coupling reaction. Shibata, Takanori; Ohta, Toshihiro; Soai, Kenso (Department of Applied Chemistry, Faculty of Science, Science University of Tokyo, Tokyo, 162-8601, Japan). Tetrahedron Letters, 39(32), 5785-5788 (English) 1998. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier Science Ltd.. Dicobalt carbonyl complex mediates an intermol. carbonylative coupling reaction between alkynylsilanes. The reaction proceeds under atmospheric pressure of argon and directly provides free cyclopentadienones in high yields (up to 99%).

IT 212125-17-2P 212125-18-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 212125-17-2 HCAPLUS

AB

CC 24-4 (Alicyclic Compounds)
Section cross-reference(s): 29

IT 212125-14-9P 212125-15-0P 212125-16-1P212125-17-2P 212125-18-3P 212125-19-4P 212125-20-7P 212125-21-8P 212125-22-9P 212125-23-0P 212125-24-1P 212125-25-2P 212125-26-3P 212125-32-1P 212125-33-2P 212125-34-3P

212125-35-4P 212125-36-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

L23 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
1971:100162 Document No. 74:100162 Reaction of triphenylsilyl halides
with sodium naphthalenide. Young, John Colin; Fearon, F. W. G.
(Edward Davies Chem. Lab., Univ. Coll. Wales, Aberystwyth, UK).
Journal of the Chemical Society [Section] B: Physical Organic (2),
272-6 (English) 1971. CODEN: JCSPAC. ISSN: 0045-6470.

AB Ph3SiCl and Ph3SiF reacted with Na naphthalenide to give 50-90%(Ph3Si)2, 1.6-90% 1,4-bis(triphenylsilyl)-1,4-dihydronaphthalene (I), and other products. The yield of I was increased in the presence of excess free naphthalene. The initial step, may involve an electron transfer mechanism to produce a triphenylsilyl radical. I was also obtained from the reaction of naphthalene and Ph3SiH in the presence of tert-Bu2O2.

IT 31027-64-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)
RN 31027-64-2 HCAPLUS
CN Silane, (1,4-dihydro-1,4-naphthylene)bis[triphenyl- (8CI) (CA INDEX NAME)

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Les Henderson